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(54) Title: RECEPTOR MODULATORS

(57) Abstract: Method of identifying a modulator of CD28 comprising comparing a structural model of a candidate modulator with a structural model of CD28 to thereby determine whether the modulator will bind to CD28, wherein the structural model is derived from, or comprises, structural coordinates of a crystal of: (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii).

RECEPTOR MODULATORS

Field of the Invention

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The present invention relates to use of a crystal structure to obtain modulators of a cell surface receptor and to the generation of therapeutic antibodies and chimeric proteins that bind a particular class of signalling receptors.

Background of the Invention

CD28 is present on the surface of T cells and plays an important role in their activation. Signal transduction occurs through CD28 after it is activated (triggered) by binding to its ligand. CD28 activation is dependent on phosphorylation of its cytoplasmic domain. CD28 does not have intrinsic phosphorylation activity but instead is dependent on an extrinsic kinase, e.g. p56lck.

Summary of the Invention

The invention relates to the obtaining of the structure of CD28. This was done by crystallizing a CD28/Fab fragment complex, subjecting it to X-ray diffraction and deriving the structural coordinates from the diffraction measurements. The Fab fragment is from an antibody that has superagonist activity towards CD28, i.e. is able to cause activation of CD28 without the need for a T cell receptor-derived signal. Conventional antibodies that activate CD28 need an additional signal generated by the T cell receptor. The deduced structure allows modulators of CD28 signalling to be obtained which can in turn be used to modulate the immune system.

Accordingly the invention provides a method of identifying a modulator of CD28 comprising comparing a structural model of a candidate modulator with a structural model of CD28 to thereby determine whether the modulator will bind to CD28, wherein the structural model is derived from, or comprises, structural coordinates of a crystal of: (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii).

In addition the invention relates to antibodies and chimeric proteins that are capable of being superagonists of particular receptors by preferentially excluding phosphatases (as opposed to kinases) from the vicinity of the said receptor.

Accordingly the invention provides an antibody that causes superagonistic signalling of a cell surface receptor, wherein said antibody binds to the extracellular portion of the receptor at a membrane proximal region and said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, wherein said antibody does not bind only the C'-D loop of human CD28.

In addition the invention provides a chimeric protein that causes superagonistic signalling of a cell surface receptor, which chimeric protein comprises (i) sequence representing a fragment of a ligand of the receptor, or a homologue of such a fragment, wherein the fragment or homologue is capable of binding to the extracellular portion of the receptor at a membrane proximal region, and (ii) an Fc region of an antibody, wherein said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.

Further the inventión provides a chimeric protein that causes superagonistic signalling of a first cell surface receptor, which chimeric protein comprises two Fv regions of an antibody that may be the same or different, wherein at least one of the Fv regions is capable of binding to said first receptor, and the other Fv region binds to a second cell surface receptor expressed on another cell, wherein said first receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, and the first receptor can be identical to the second receptor.

Description of the drawings

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Figure 1 shows mechanisms of differential triggering of extrinsic kinase-dependent receptors, by superagonistic agents *in vitro* and in *vivo*.

A. In vitro superagonistic signalling, giving the example of CD28 antibodies. The basic signalling principle is as follows. Antibodies raised against CD28 bind distally ("conventional" antibodies, left) or membrane-proximally ("superagonists", right), as indicated by the structure of the CD28-5.11A1 antibody-Fab complex. The antibodies hold the cell surface at certain distances from an immobilising substrate: in this case plastic, and as shown in parts B, C and D of the figure, Fc receptor- or other receptor-bearing cells. For superagonistic antibodies this distance is typically 150-200Å, whereas for costimulatory antibodies, it is considerably larger.

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The induced proximity of the membrane and the immobilising substrate in the region of the immobilised antibody and receptor will lead to the differential steric exclusion, from the immediate vicinity of the receptor, of other molecules whose extracellular domains are comparable in size or larger than CD28-antibody complexes, such as the tyrosine phosphatase, CD45. In contrast, tyrosine kinases, e.g. p56lck, will be unaffected because they are small and/or attached to the inner leaflet of the membrane. The result is that, overall, the phosphorylation of CD28 by the kinases will be favoured over its de-phoshorylation by phosphatases, with the net increase in phosphorylation amounting to receptor triggering. Superagonists are more potent than conventional antibodies because they bind epitopes close to the membrane rather than at the "top" of the molecule, leading to more efficient exclusion of, e.g., CD45, and therefore a larger increase in the net phosphorylation of CD28.

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B. In vivo superagonistic signalling, giving the example of CD28 antibodies. The binding of the antibody to the membrane-proximal region of CD28 on a T cell, and to the Fc receptor of, e.g. an antigen presenting cell, forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of CD28 as described in A, leading to signalling by CD28.

C. In vivo superagonistic signalling, giving the example of a chimeric, ligand-based agent. The chimera consists of a receptor-binding region of the ligand of the receptor, fused to the Fc region of an antibody. The binding of the ligand portion of the chimera to the receptor, and of the Fc region of the chimera to the Fc receptor of, e.g. an antigen presenting cell, forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of the receptor as described in A, leading to signalling by the receptor.

D. In vivo superagonistic signalling, giving the example of a chimeric, Fv-based agent. The chimera consists of the receptor-binding Fv region of one antibody, fused to the Fv region of a second antibody reactive with another receptor on a second cell. The binding of the chimera to both receptors forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of the receptor as described in A, leading to signalling by the receptor.

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Figure 2 shows the method for identification of binding sites for superagonist antibodies of receptors raised against example receptors.

Description of the sequences mentioned herein

SEQ ID NO:1 shows the amino acid sequence of CD28.

SEQ ID NO:2 shows the sequence of the CD28/Fc fusion protein used to express and dimerise CD28.

Detailed description of the invention

10 The CD28 protein

Many of the different aspects of the invention discussed herein refer to CD28. It is to be understood that references to CD28 herein also include (i) a homologue of CD28, or (ii) a fragment of CD28 or the homologue, or (iii) a fusion protein comprising CD28, (i) or (ii), unless the context requires otherwise. The homologue and/or fragment of CD28 may be of particular lengths, as discussed below, or may have the binding or functional properties of naturally occurring (native) CD28, such as the ability to bind a cell membrane and/or bind to B7-1 or B7-2. The homologue and/or fragment may comprise the extracellular domain of CD28. The homologue and/or fragment may comprise, or essentially consist of, the fragment of CD28 present in the fusion protein of SEQ ID NO:2. The homologue and/or fragment may have the ability to transduce a signal to the cytoplasm of a T cell.

The CD28 may be of any species of animal, such as a mammalian or avian CD28. The CD28 is preferably a human CD28, for example as shown in SEQ ID NO:1. The CD28 protein may be present in particular forms, for example which aid expression and/or crystallization. Thus the CD28 may be fully glycosylated, partially glycosylated or lack glycosylation and/or have a reduced and alkylated stalk region.

The CD28 crystal

The crystal of CD28 generally comprises CD28 present in a regular repeating array. As mentioned above the term "CD28" includes fragments and/or homologues. Preferred fragments or homologues present in the crystal comprise the extracellular

domain of native CD28. In the crystal the CD28 is preferably in the form of a monomer. The crystal may be of CD28 bound to another moiety. Such a moiety may be an antibody specific for CD28, including fragments/ derivatives of the antibody (as further discussed below), which bind CD28. In a preferred embodiment the crystal is of CD28 bound to the Fab fragment of an antibody. The crystal may comprise CD28 in a form that aids crystallization, and thus the CD28 may be fully glycosylated, partially glycosylated or lack glycosylation and/or have a reduced and alkylated stalk region. In one embodiment the crystal has the coordinates shown in Table 4.

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The crystal is generally obtained by providing a solution that comprises CD28 and optionally a moiety that binds to CD28, such as an antibody fragment, and subjecting the solution to conditions that allow the crystal to form. The CD28 which is to be crystallized is generally obtained by recombinant expression, optionally in the form of a fusion protein. The fusion protein may comprise CD28 and a polypeptide sequence which forms a homodimer. Such a fusion protein aids the formation of a CD28 homodimer. Preferably the fusion protein comprises the sequence of the Fc region of an antibody. The fusion protein may be cleaved before crystallisation to separate CD28 from the other polypeptide sequence, for example by thrombin.

The CD28 may be expressed in any suitable cell that is able to express large amounts of CD28, such as a Chinese hamster ovary (CHO) cell.

The CD28 may be further treated in order to aid crystallization. Binding to an antibody fragment, such as a Fab fragment, may be used to prevent the N-linked glycans present on the fully glycosylated form of CD28 from inhibiting the crystallisation of the protein. In one embodiment the antibody (or fragment thereof) is a superagonistic antibody, which may have any of the properties of the superagonistic antibodies mentioned herein. Thus, in one embodiment the antibody (or fragment thereof) binds to a loop region in the extracellular membrane proximal region of CD28, such as the C'-D loop (said loop being defined for example as defined in US-A1-2003/0166860 as the sequence from amino acid positions 52 to 66 CD28 represented by the sequence GNYSQQLQVYSKTGF).

The treatment may comprise reduction of the interchain disulphide bonds in the stalk-like region of CD28, e.g. using dithioreitol (DTT). The reduced cysteines may then be inactivated, for example by alkylation (typically the alkyl moiety has 2 to 6, preferably 2, carbons). The alkylation may be performed using iodoacetamide.

Crystallisation is typically carried out at 15 to 25°C, such as at 17 to 19°C, preferably 18°C. Magnesium formate and polyethylene glycol (PEG) may be used as precipitating agents. Preferably precipitation is carried out using 0.15 to 0.25 M magnesium formate (such as 0.2 M magnesium formate) and 15 to 25 % PEG 3350 (such as 20% PEG 3350).

In the work described in the Examples it was found that in order to crystallise CD28 this protein had to be expressed in the form of a fusion protein with a second protein capable of forming a homodimer (the Fc region of an antibody), the fully glycosylated form of CD28 needed to be complexed with an Fab fragment of an antibody in order that the N-linked glycans did not interfere with crystallisation, and the disulphide bonds in the stalk region of CD28 needed to be reduced and alkylated so that the stalk did not interfere with crystallisation. Thus in a preferred embodiment the method of obtaining a crystal of CD28 (including fragment and/or homologue thereof) comprises

- (a) expressing CD28 in the form of a fusion protein with a second protein that is able to form a homodimer, wherein the presence of the second protein in the fusion protein causes CD28 to dimerise,
 - (b) cleaving the second protein from the fusion protein,
- (c) reducing and alkylating the disulphide bond present in the stalk-like region of CD28, and
- (d) crystallising CD28 bound to the Fab fragment of an antibody.

Identifying a modulator of CD28

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The invention provides a method of identifying a modulator using the structural coordinates determined from the above-mentioned crystal of CD28. The structural coordinates used in the method may be in the form of a structural model, such as a three dimensional representation of the structure or a pharmacophore. The coordinates/model typically comprise information relating to the identity of each

atom (i.e. whether it is nitrogen, oxygen, hydrogen etc.) and its three dimensional location (normally defined by three spatial coordinates) in the structure. The model may also comprise additional information relevant to obtaining modulators, such as the electronic charge at different locations in the structure or information concerning whether or not the bonds in the structure can be rotated.

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The coordinates/model used in the method typically comprise a specific region of the surface of CD28 corresponding to the site where it is desired for the modulator to bind. Such a site typically comprises Glu-32, Arg-34, Tyr-51, Glu-97, Met-99, Tyr-100, Pro-101, Pro-102, Pro-103, Tyr-104 and Leu-105, or a part thereof which comprises one or more of these amino acids. Preferred modulators bind to such a site or part thereof. In one embodiment the modulator is able to inhibit binding of another moiety to this site. Such a moiety may be an antibody which is specific to the site.

In the method the coordinates/model of CD28 are compared to the structural coordinates/model of a candidate modulator to determine whether or not the candidate modulator will bind to CD28. The comparison may be performed by any suitable means, such as the methods described or referenced in Lyne (2002) Drug Discovery Today 7, 1047-1055. Thus one or more of the algorithms described in this document may be used, such as one or more of Dock, FlexX, FlexE, Slide, Fred, Gold, Glide, AutoDock, LigandFit, ICM, QXP, Amber, CHARMM, SCORE, VALIDATE, Chemscore, Ludi, PLP, PMF, Bleep, SmoG, ZAP, VIDA, GRID, MCSS, Superstar and ROCS.

The method typically comprises deducing one or more ways of fitting (docking) a candidate modulator with CD28 followed by an evaluation (scoring) of the fit. The evaluation may comprise deducing the binding energy between CD28 and the modulator. This may be done based on the interatomic distances between the atoms involved in binding or by analysis of the force fields of CD28 and the modulator. In one embodiment the evaluation comprises comparing the similarity between the fit between CD28 and the candidate modulator and the fit between one or more other proteins and their ligands. Thus the evaluation may comprise comparison with a database of structures of proteins fitted/bound to ligands.

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A candidate modulator which has been selected computationally as discussed above may be physically tested to determine whether or not it is able to bind or modulate CD28. Any suitable binding or activity assay may be used. The binding assay may measure the extent of direct binding between the candidate modulator and CD28 or instead be in the form of a competition assay. The binding assay may comprise/use of any of the following:

- (a) an assay of binding to CD28 (which may be immobilized), for example in which
- (i) the inhibition of B7-1 binding to the CD28 (a soluble form of B7-1 may be used) in the presence of the candidate modulator is measured,
- (ii) inhibition of the binding of an antibody (that binds to the ligand binding face of CD28) to the CD28 in the presence of the candidate modulator is measured,
 - (b) a scintillation proximity assay (SPA) in which (i) or (ii) above are measured,
 - (c) an ELISA assay in which (i) or (ii) above are measured.

The activity assay may test the effect of the candidate modulator on the ability of B7-1 or B7-2 to activate CD28. In such an assay, B7-1 or B7-2 may be present on a natural or artificial antigen-presenting cell and CD28 may be present on a T cell. CD28 activity may be detected by measuring the extent of T cell activation, for example by determining the extent of T cell proliferation (e.g. thymidine incorporation) or gene expression in the T cell (e.g. with microarrays).

The candidate modulator may be tested using the assays described in Green NJ, Xiang J, Chen J, Chen L, Davies AM, Erbe D, Tam S, Tobin JF. (2003) Structure-activity studies of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones binding to the immune regulatory protein B7.1. Bioorg Med Chem. 11, 2991-3013 or Erbe DV, Wang S, Xing Y, Tobin JF. (2002) Small molecule ligands define a binding site on the immune regulatory protein B7.1. J Biol Chem. 277, 7363-8.

The antibody and chimeric protein of the invention

The term "antibody" as used herein is understood to also include fragments and derivatives of the antibody which retain binding ability, unless the context requires otherwise. Such fragments/derivatives include Fv, F(ab') and F(ab')₂ fragments, as well as single chain antibodies, camelid antibodies and similarly acting proteins.

The antibody of the invention may be of any species, such as a mammalian or bird antibody, preferably a rodent (such as mouse) or primate (such as human) antibody. The antibody may be a chimeric antibody, a CDR-grafted antibody or a humanised antibody. The antibody may be monoclonal or polyclonal. The antibody is preferably an IgG antibody.

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The invention also provides two types of chimeric protein that bind to a receptor. One type of chimeric protein comprises the sequence of a fragment of a ligand of the receptor, or sequence that is homologous to such a fragment. The sequence is capable of binding to an extracellular region of the receptor, as discussed further below. The chimeric protein also comprises the Fc region of an antibody, such as that of any of the types of antibody discussed above. Where the chimeric protein is administered to an individual the Fc region may be of an antibody of the same species as the individual.

The second type of chimeric protein provided by the invention comprises two Fv regions of an antibody. The Fv regions may be the same or different. One of the Fv regions is capable of binding to the extracellular region of the receptor (the "first" receptor). The other Fv region may bind the extracellular region of a "second" apposing receptor, this being the same type of receptor as the first receptor (with the second Fv binding at a location which is the same or different from the first Fv region) or an entirely different cell surface receptor, for example in the case where the first and second receptors are each expressed on the surfaces of two cells capable of interacting/contacting each other. Such cells may be any of the types of cell mentioned herein, including T cells.

In one embodiment the second Fv region of the second type of chimeric protein binds to a protein expressed on the surface of T cells, such as the T cell receptor, CD2, CD4, CD5, CD8, CD52 or CS1. The second Fv region may bind proteins expressed on the surface of other cells, such as CD48, CD58, CD59, B7-1 or B7-2. The term "receptor" when used in the present context refers to a protein expressed on surface of a cell (which may or may not be one which is capable of signal transduction, for example).

The antibody and chimeric protein of the invention are able to cause superagonistic signalling of a cell surface receptor when they bind to the receptor,

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typically according to the mechanism illustrated in Figure 1. Thus the antibody or chimeric protein is able to cause activation of the receptor (i.e. cause the receptor to transduce a signal to the cytoplasm of the cell) without the need for additional costimulus of the receptor or cell. As mentioned above, in one embodiment the second type of chimeric protein comprises Fv regions able to bind to different types of receptors. Such a chimeric protein is preferably able to induce superagonistic signalling by both of the receptors which it binds.

The antibody and both types of chimeric protein bind the extracellular portion of the receptor at a membrane proximal region of the receptor, typically to a region of the receptor which is within 75Å of the cell membrane, such as within 60Å, 50Å or 40Å of the cell membrane. However the second type of chimeric protein of the invention typically also binds the extracellular portion of the second apposing receptor (as defined above), within 75Å of the cell membrane, such as within 60Å, 50Å or 40Å of the cell membrane.

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Generally the antibody or chimeric protein will be capable of binding the native form of the receptor (at the extracellular regions discussed above) when the receptor is present on the surface of the cell where it occurs naturally.

The antibody or chimeric protein cause superagonistic signalling by sterically hindering the access of phosphatases (which tend to be large proteins), such as CD45, to the receptor (i.e. hindering contact of the phosphatase and receptor). In the case of the antibody or first type of chimeric protein such steric hindrance may be caused by the antibody binding to the receptor at one end (through the Fab of the antibody of the invention or the ligand sequence of the first type of chimeric protein) and typically binding to a protein on the surface of another cell (e.g. due to the Fc region of the antibody or chimeric protein binding to an Fc receptor expressed on a second cell), thus bringing the cell membrane of the two cells into close proximity in the region of the receptor.

For the second type of chimeric protein, one of the Fv fragments of the chimeric protein will bind to the receptor, and in the case where the other Fv fragment is specific for a second type of receptor expressed on another cell, the other Fv fragment will bind to the second receptor and thus bring the cell membranes of the two cells into close proximity in the region of the first receptor.

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For the antibody and both types of chimeric protein, the close proximities of the cell membranes in the region of the first receptor will sterically hinder phosphatases from accessing the receptor, leading to signal transduction or "triggering" of the receptor. The antibody or chimeric protein are typically capable of bringing the cell membranes of two cells within 200Å of each other, such as within 180Å, 150Å or 120Å of each other.

The antibody or chimeric protein will preferably bind orthogonally to the main axis of the domain of the receptor which is bound, such as at more than 60 degrees from the main axis of the bound domain of the receptor, for example at more than 70, 80 or 90 degrees. The antibody or chimeric protein will preferably lie substantially parallel to the cell surface when bound to the receptor (to ensure the membranes are brought into close proximity).

The antibody or chimeric protein will bind to an extracellular region of the receptor, generally to amiño acids of the receptor that are exposed at the surface of the protein. The amino acids in the receptor that are bound may be present in a loop region or a β -strand of the receptor. Preferred loops and strand sequences are shown for key examples in Table 1. The antibody or chimeric protein may bind to any of the epitopes or part thereof shown in Table 1 or an equivalent homologous sequence from the membrane proximal region of other receptors.

The antibody of the invention does not bind only to the C'-D loop of CD28, and thus in one embodiment will bind both the C'-D loop of CD28 and another region of CD28. The antibody may be one which does not bind any portion of the C'-D loop of CD28. The antibody may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The antibody of the invention may or may not bind to any or all of the sequences shown in Table 3.

The first type of chimeric protein of the invention may or may not bind to only the C'-D loop of CD28. The first type of chimeric protein may be one which does not bind to any portion of the C'-D loop of CD28. The first type of chimeric protein may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The first type of chimeric protein may or may not bind to any or all of the sequences shown in Table 3.

The second type of chimeric protein of the invention may or may not bind to

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only the C'-D loop of CD28. The second type of chimeric protein may be one which does not bind to any portion of the C'-D loop of CD28. The second type of chimeric protein may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The second type of protein may or may not bind to any or all of the sequences shown in Table 3.

Receptors bound by the antibody and chimeric protein

The receptors which are bound by the antibody or chimeric protein of the invention are expressed on the cell surface. The receptor is capable of being phosphorylated (typically at one or more tyrosine residues in the cytoplasmic region of the receptor), and phosphorylation of the receptor will typically lead to its activation. The receptor will comprise a cytoplasmic domain that is dependent on extrinsic protein kinases to be phosphorylated. Thus the receptor will not have an intrinsic enzymatic (kinase or phophatase) activity. The receptor will typically comprise tyrosine-containing, activating ITAM motifs (YxxL/Ix₇₋₁₂YxxL/I), inhibitory ITIM motifs (I/V/L/SxYxxL/V) or "switch" (TxYxxV/I; activating and inhibitory) signalling motifs (where x is any amino acid). These motifs are phosphorylated by cytoplasmic tyrosine kinases, such as the Src kinases, in competition with antagonistic tyrosine phosphatases, such as CD45. The signalling character of the receptors is defined exclusively by the nature of these motifs (ITAM vs ITIM: activating vs inhibitory).

The receptor may be a member of any surface protein superfamily, but is typically a member of the immunoglobulin superfamily. The receptor may be a member of the CD28 superfamily. The receptor may be any of the specific receptors which are shown in Table 1 or 2 or may comprise a sequence which is homologous to the sequence of any of these specific receptors. The receptor may be CD28, CTLA-4, ICOS, PD-1 or BTLA or comprise a sequence which is homologous to the sequence of any of these specific receptors.

The receptor may be of any of the species that are mentioned herein, and thus may be a mammalian or avian, preferably rodent (such as mouse or rat) or primate (such as human) receptor.

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The receptor may be naturally present on a cell of the immune system such as a T cell, B cell, myeloid cell, mast cell, NK cell or a granulocyte.

Screening methods of the invention

The invention provides a method of obtaining an agent which is capable of superagonising the above-mentioned receptor which binds to the antibody and chimeric protein of the invention. The method comprises determining whether a candidate agent has any of the properties discussed above possessed by the antibody or chimeric protein of the invention which allows them to induce superagonistic signalling by a receptor. Thus the method will generally comprise determining whether a candidate agent is able to bind to an extracellular membrane proximal region of the receptor, and may also determine whether a candidate agent is able to bind

- at a particular location from the cell membrane (such as within 75Å of the cell membrane),
- to particular sequences (such as the sequences mentioned in Table 1), or
- in a manner (such as orthogonal to the main axis of the bound receptor domain) which is discussed above for binding of the antibody or chimeric protein of the invention.

Suitable extracellular membrane proximal regions of a receptor may be identified using a sequence database search algorithm (e.g. BLAST) to search for the solved structure most related to the receptor in the protein structural database (PDB). This structure would then be used to identify membrane proximal regions (preferably β-strands) in the receptor by sequence alignment. Whether or not a candidate agent binds to the identified sequences could be determined by taking the midpoint of the strand and the side chains of amino acids two- and three-residues below this midpoint could then be mutated. Mutant forms of the receptor mutated at each of these residues would then be expressed (e.g. on suitable target cells that can be transfected stably or transiently, such as 293T cells), and used to screen for candidate agents that bound the non-mutated receptor but failed to bind the mutant receptor, for example using fluorescence-activated cell sorting. It is envisaged that only every second strand in a conventional beta barrel protein would need to be mutated. In the case of

PD-1 protein, which is representative of receptors not related to CD28.

a receptor which is a member of the immunoglobulin superfamily, this corresponds to 8-10 mutant lines being generated, in total. Examples of this process are shown in Figure 2 for the immediate CD28 family members (ICOS and CTLA-4) and for the

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Agents that induce superagonistic signalling by a receptor may also be identified using a peptide which comprises sequence from the extracellular membrane proximal region of a receptor or homologous sequence thereto. Such a sequence is typically 5 to 20 amino acids long, such as 10 to 15 amino acids long. In one embodiment the agent is identified using peptide arrays. The mapping of discontinuous epitopes can be performed using overlapping peptides derived from the entire primary sequence of a protein. The whole protein sequence is generated in the form of short overlapping peptides (for example each shifted by 3 amino acids), e.g. prepared by standard spot synthesis (Automated Spot Synthesiser, Abimed, Langenfeld, Germany) on Whatman 50 filter paper (Whatman, Maidstone, England). The C-termini of the peptides may be attached to cellulose via a (β-Ala)₂ spacer and the N-termini acetylated. The arrays may be subsequently probed either directly on the peptide membrane or after transfer to another surface (e.g. nitrocellulose) using the monoclonal antibody and a chemiluminescence-based detection system (ECL Western Blotting Detection System, Amersham Pharmacia Biotech).

Suitable candidate agents that can be tested in the above screening methods include antibody agents (for example, monoclonal and polyclonal antibodies, single chain antibodies, chimeric antibodies and CDR-grafted antibodies). Furthermore, combinatorial libraries, defined chemical identities, peptide and peptide mimetics, oligonucleotides and natural agent libraries, such as display libraries (e.g. phage display libraries) may also be tested. The candidate agents may be chemical compounds, which are typically derived from synthesis around small molecules. Batches of the candidate agents may be used in an initial screen of, for example, ten substances per assay, and the agents of batches which show the required property tested individually.

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Obtaining a superagonistic antibody

The invention provides methods for obtaining a superagonistic antibody. In one embodiment the method comprises screening antibodies for the ability to superagonise a receptor, wherein the antibodies have been obtained either by immunizing an animal with the receptor or a homologue or fragment of the receptor, or from a combinatorial antibody library. Preferably the animal is immunized with a protein which comprises the sequences shown in Table 1, or a fragment thereof, or a homologue of such a sequence or fragment.

Whether or not an antibody is a superagonistic antibody may be ascertained by determining whether or not the antibody can bind an extracellular membrane proximal region of a receptor, for example using any of the suitable methods described above in the section of screening for superagonistic agents.

Alternatively the antibody can be tested in an activity assay to see whether or not it causes activation of the receptor. Receptors that are activated by the antibody will either transduce an activating signal or an inhibitory signal to the cell cytoplasm. In the case of receptors which transduce an activating signal, as in the case of CD28, the activity which is tested may be activation of the cell. This can be determined using functional screens based on, for example, cell proliferation, increased cellular calcium, enhanced tyrosine phosphorylation of proteins in the cell or the production of/release of substances by the cell, e.g. IL-2 production. In the case of receptors that transduce inhibitory signals when activated, activation of such receptors can be ascertained by detection of any of the changes which occur to the receptor or the cell when such a signal is transduced, such as changes in the extent of phosphorylation of one or more proteins in the cell.

The binding or activity assay may be carried out in vitro (inside or outside a cell) or in vivo.

In one embodiment of the method the antibody is obtained by immunising an animal with a peptide comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor, or a homologue of such sequence, and obtaining the antibody produced by the animal against said sequence. Alternatively the antibody may be obtained by selecting an antibody from a combinatorial library based on its ability to bind a peptide

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comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor, or a homologue of such sequence.

In one embodiment the peptide which is used to immunise the animal or select an antibody from a library only comprises sequence from the receptor, or a homologue thereof, and does not comprise any additional sequence. In this embodiment the peptide will only be 5 to 20 amino acids long. However in other emobodiments the peptide comprises other sequence to the N-terminus and/or C-terminus of the receptor sequence, such as sequence which is different from (and typically not homologous to) receptor sequence.

Antibodies

Various types of antibodies are mentioned herein, including antibodies obtained by immunisation. Such antibodies may be raised against specific epitopes/sequences. An antibody, or other compound, "specifically binds" to a sequence when it binds with preferential or high affinity to the sequence for which it is specific but does not bind or binds with only low affinity to other sequences. A variety of protocols for competitive binding or immunoradiometric assays to determine the specific binding capability of an antibody are well known in the art (see for example Maddox *et al*, J. Exp. Med. <u>158</u>, 1211-1226, 1993). Such immunoassays typically involve the formation of complexes between the specific sequence and its antibody and the measurement of complex formation.

Means for preparing and characterising antibodies are well known in the art, see for example Harlow and Lane (1988) "Antibodies: A Laboratory Manual", Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY. For example, an antibody may be produced by raising antibody in a host animal.

A method for producing a polyclonal antibody comprises immunising a suitable host animal, for example an experimental animal, with the immunogen and isolating immunoglobulins from the animal's serum. The animal may therefore be inoculated with the immunogen, blood subsequently removed from the animal and the IgG fraction purified.

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A method for producing a monoclonal antibody comprises immortalising cells which produce the desired antibody. Hybridoma cells may be produced by fusing spleen cells from an inoculated experimental animal with tumour cells (Kohler and Milstein (1975) *Nature* **256**, 495-497).

An immortalized cell producing the desired antibody may be selected by a conventional procedure. The hybridomas may be grown in culture or injected intraperitoneally for formation of ascites fluid or into the blood stream of an allogenic host or immunocompromised host. Human antibody may be prepared by *in vitro* immunisation of human lymphocytes, followed by transformation of the lymphocytes with Epstein-Barr virus.

For the production of both monoclonal and polyclonal antibodies, the experimental animal is suitably a goat, rabbit, rat, mouse, guinea pig, chicken, sheep or horse. If desired, the immunogen may be administered as a conjugate in which the immunogen is coupled, for example via a side chain of one of the amino acid residues, to a suitable carrier. The carrier molecule is typically a physiologically acceptable carrier. The antibody obtained may be isolated and, if desired, purified.

The peptide of the invention

The invention also provides a peptide of length 5 to 20 amino acids comprising a sequence which binds to the superagonistic antibody of the invention. The peptide may have a length of 10 to 15 amino acids. The peptide may comprise sequence from an extracellular membrane proximal region of any of the receptors mentioned herein or have a homologous sequence thereto (such sequence may have a length of 5 to 20 amino acids). The peptide may thus comprise any of the sequences shown in Table 1 or homologues of such sequences.

Therapeutic aspects of the invention

The invention provides substances which can be used to treat a patient. The patient is typically a human or animal, such as a mammal or bird, for example a cow, sheep, goat, pig, camel, horse, dog, cat, goosè, duck or chicken.

The modulator of CD28 which is identified from a structural model or structural coordinates of CD28 can be used to modulate the immune system of a

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patient. Such modulators will either agonise or antagonize CD28 (i.e. cause or contribute to an increase or decrease, respectively, in CD28 signalling activity). Modulators which agonise CD28 may be used to stimulate the activity of T cells (which express CD28) and thus to stimulate an immune response against an antigen. Such modulators may therefore be used in the prevention or treatment of a disease caused by a pathogenic agent, such as a virus, microorganism (for example a bacterium) or multicellular organism; or in the prevention or treatment of a cancer.

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Modulators which antagonise CD28 may be used to inhibit the activity of T cells, and thus to inhibit an immune response to an antigen. Such modulators may be used to prevent or treat an autoimmune disease (such as rheumatoid arthritis or asthma), allergy or transplantation rejection.

The superagonistic antibodies, chimeric proteins and agent described herein may also be used in the therapy of patients to prevent or treat a disease. These substances may be used to modulate the state of a cell on which the relevant receptor is present. Thus the substance may activate or inhibit cell activity depending on whether the activated receptor transduces a stimulatory or inhibitory signal to the cytoplasm of the cell. The modulation of the cell may thus be used to treat a disease caused by the cell or a disease which can be alleviated or prevented by the cell.

In a preferred embodiment the cell is a cell of the immune system (e.g. any such cell mentioned herein) and therefore superagonistic antibodies, chimeric proteins and agents may be used to modulate the immune response of a patient. Superagonistic antibodies, chimeric proteins and agents which stimulate an immune response may be used in the prevention or treatment of a disease caused by a pathogenic agent, such as a virus, microorganism (for example a bacterium) or multicellular organism; or in the prevention or treatment of a cancer. Superagonistic antibodies, chimeric proteins and agents which inhibit an immune response may be used to prevent or treat an autoimmune disease (such as rheumatoid arthritis or asthma), allergy or transplantation rejection.

The patient may also be treated by generating a superagonistic antibody response in the patient by immunisation with a peptide that stimulates the generation of such a response. The antibody that is generated will be specific to a sequence present in the peptide. The peptide will comprise sequence from the extracellular

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membrane proximal region of a receptor, or sequence which is homologous thereto. Such receptor sequence may be any of the membrane proximal sequences of a receptor (or homologues thereof) mentioned herein. Thus the peptide may be any of the peptides mentioned herein which comprise such sequence.

In one embodiment a nucleic acid capable of expressing any of the abovementioned therapeutic substances is administered to the patient. Such a nucleic acid typically comprises a region which encodes the therapeutic substance and a control region which causes expression of the coding sequence, such as a promoter. Thus the nucleic acid may be in the form of a vector.

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The substances mentioned herein

The modulators, antibodies, chimeric proteins, peptides and nucleic acids mentioned herein may be present in a substantially isolated form. They may be mixed with carriers or diluents which will not interfere with their intended use and still be regarded as substantially isolated. They may also be in a substantially purified form, in which case they will generally comprise at least 90%, e.g. at least 95%, 98% or 99%, of the proteins nucleic acids or dry mass of the preparation.

Homologues

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Homologues of protein sequences are referred to herein. Such homologues typically have at least 50% homology, preferably at least 60%, 70%, 80, 90%, 95%, 97% or 99% homology, for example over a region of at least 15, 20, 30, 100 more contiguous amino acids. The homology may be calculated on the basis of amino acid identity (sometimes referred to as "hard homology").

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For example the UWGCG Package provides the BESTFIT program which can be used to calculate homology (for example used on its default settings) (Devereux et al (1984) Nucleic Acids Research 12, p387-395). The PILEUP and BLAST algorithms can be used to calculate homology or line up sequences (such as identifying equivalent or corresponding sequences (typically on their default settings), for example as described in Altschul S. F. (1993) J Mol Evol 36:290-300; Altschul, S, F et al (1990) J Mol Biol 215:403-10.

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Software for performing BLAST analyses is publicly available through the National Center for Biotechnology Information (http://www.ncbi.nlm.nih.gov/). This algorithm involves first identifying high scoring sequence pair (HSPs) by identifying short words of length W in the query sequence that either match or satisfy some positive-valued threshold score T when aligned with a word of the same length in a database sequence. T is referred to as the neighbourhood word score threshold (Altschul et al, supra). These initial neighbourhood word hits act as seeds for initiating searches to find HSPs containing them. The word hits are extended in both directions along each sequence for as far as the cumulative alignment score can be increased. Extensions for the word hits in each direction are halted when: the cumulative alignment score falls off by the quantity X from its maximum achieved value; the cumulative score goes to zero or below, due to the accumulation of one or more negative-scoring residue alignments; or the end of either sequence is reached. The BLAST algorithm parameters W, T and X determine the sensitivity and speed of the alignment. The BLAST program uses as defaults a word length (W) of 11, the BLOSUM62 scoring matrix (see Henikoff and Henikoff (1992) Proc. Natl. Acad. Sci. USA 89: 10915-10919) alignments (B) of 50, expectation (E) of 10, M=5, N=4, and a comparison of both strands.

The BLAST algorithm performs a statistical analysis of the similarity between two sequences; see e.g., Karlin and Altschul (1993) *Proc. Natl. Acad. Sci.* USA 90: 5873-5787. One measure of similarity provided by the BLAST algorithm is the smallest sum probability (P(N)), which provides an indication of the probability by which a match between two amino acid sequences would occur by chance. For example, a sequence is considered similar to another sequence if the smallest sum probability in comparison of the first sequence to the second sequence is less than about 1, preferably less than about 0.1, more preferably less than about 0.01, and most preferably less than about 0.001.

The homologous sequence typically differs by at least 1, 2, 5, 10, 20 or more mutations (each of which may be a substitution, deletion or insertion of an amino acid). These mutations may be measured across any of the regions mentioned above in relation to calculating homology. The substitutions are preferably conservative substitutions. These are defined according to the following Table. Amino acids in

the same block in the second column and preferably in the same line in the third column may be substituted for each other:

ALIPHATIC	Non-polar	GAP
		ILV
	Polar – uncharged	CSTM
		NQ
	Polar - charged	DE
		KR
AROMATIC		HFWY

5 Administration

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The formulation of any of the therapeutic substances mentioned herein will depend upon factors such as the nature of the substance and the condition to be treated. Any such substance may be administered in a variety of dosage forms. It may be administered orally (e.g. as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules), parenterally, subcutaneously, intravenously, intramuscularly, intrasternally, transdermally or by infusion techniques. The substance may also be administered as suppositories. A physician will be able to determine the required route of administration for each particular patient.

Typically the substance is formulated for use with a pharmaceutically acceptable carrier or diluent. The pharmaceutical carrier or diluent may be, for example, an isotonic solution. For example, solid oral forms may contain, together with the active compound, diluents, e.g. lactose, dextrose, saccharose, cellulose, corn starch or potato starch; lubricants, e.g. silica, tale, stearic acid, magnesium or calcium stearate, and/or polyethylene glycols; binding agents; e.g. starches, arabic gums, gelatin, methylcellulose, carboxymethylcellulose or polyvinyl pyrrolidone; disaggregating agents, e.g. starch, alginic acid, alginates or sodium starch glycolate; effervescing mixtures; dyestuffs; sweeteners; wetting agents, such as lecithin, polysorbates, laurylsulphates; and, in general, non-toxic and pharmacologically

inactive substances used in pharmaceutical formulations. Such pharmaceutical preparations may be manufactured in a known manner, for example, by means of mixing, granulating, tabletting, sugar-coating, or film coating processes.

Liquid dispersions for oral administration may be syrups, emulsions and suspensions. The syrups may contain as carriers, for example, saccharose or saccharose with glycerine and/or mannitol and/or sorbitol.

Suspensions and emulsions may contain as carrier, for example a natural gum, agar, sodium alginate, pectin, methylcellulose, carboxymethylcellulose, or polyvinyl alcohol. The suspensions or solutions for intramuscular injections may contain, together with the active compound, a pharmaceutically acceptable carrier, e.g. sterile water, olive oil, ethyl oleate, glycols, e.g. propylene glycol, and if desired, a suitable amount of lidocaine hydrochloride.

Solutions for intravenous or infusions may contain as carrier, for example, sterile water or preferably they may be in the form of sterile, aqueous, isotonic saline solutions.

A therapeutically effective amount of substance is administered. The dose may be determined according to various parameters, especially according to the substance used; the age, weight and condition of the patient to be treated; the route of administration; and the required regimen. Again, a physician will be able to determine the required route of administration and dosage for any particular patient. A typical daily dose is from about 0.1 to 50 mg per kg, preferably from about 1.0 mg per kg to 10 mg per kg of body weight, according to the activity of the specific therapeutic substance, the age, weight and condition of the subject to be treated, the type and severity of the disease and the frequency and route of administration.

The following Examples illustrate the invention:

Preferably, daily dosage levels are from 5 mg to 2 g.

Examples

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Overview of crystallisation strategy

In order to undertake crystallization trials with glycoproteins, such as the CD28 homodimer, it is generally necessary to produce large amounts of protein (>10 milligrams). For this the glutamine synthetase-based Chinese hamster ovary cell expression system (Lonza Biologics Plc, UK) was chosen, which is one of the few

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eukaryotic expression systems capable of glycoprotein production at this level. The Lec3.2.8.1 cell line was used as the expression host as this provides the option of enzymatically removing unnecessary glycosylation after protein folding and secretion has taken place, which generally favours crystallization. In order to enhance homodimerization, the protein was expressed in the form of a fusion protein with the Fc region of immunoglobulin, which is itself a homodimer. Because the link between the CD28 portion and the Fc is extremely flexible (which will generally discourage crystallization), the construct was prepared in a way that made it thrombin-cleavable.

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It was found that producing active, thrombin-cleavable protein depended on the location of the cleavage site. When the cleavage site was too close to the ligand binding domain (to make a more compact protein for crystallization), the protein produced was mis-folded.

In general removal of the N-linked glycans from a glycoprotein substantially enhances its ability to crystallise. Unexpectedly, and in marked contrast to other cell surface glycoproteins, which are generally very stable and active after deglycosylation, the CD28 homodimer proved to be very unstable after deglycosylation with the enzyme endoglycosidase H at the slightly acidic pH at which this enzyme is active. Therefore it was necessary to leave the glycosylation of CD28 intact. The glycosylated form of the homodimer failed to crystallise in more than 100 trials.

To reduce the impact of the glycosylation, therefore, an alternative strategy was employed, in which Fab fragments of anti-CD28 antibodies were prepared and crystallised with CD28. Fab fragments are almost invariably unglycosylated, so the formation of complexes with the Fab can be expected to reduce the impact of the glycans by 80%, regardless of where they bind the protein of interest (a Fab is four times the size of the CD28 monomer). The likelihood that the complex of the Fab and protein of interest will crystallise depends on the overall shape of the complex, (i.e. its "compactness") and on the chemical properties of the surfaces of the complex involved in forming crystal lattice contacts. Because the surface of the complex that will form lattice contacts cannot be predicted *a priori*, it is impossible to predict whether a given Fab will give crystals when complexed with the protein. Not unexpectedly, therefore, the homodimer still failed to crystallize after being complexed with one Fab molecule

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per homodimer for two different antibodies (5.11A1 and 9D7), or two Fabs per homodimer for one of these antibodies (5.11A1), in >100 trials per complex.

In addition the stalk region was expected to create problems. The key to obtaining crystals was to prepare monomeric CD28 by gentle reduction and alkylation of the interchain disulphide bond in the stalk-like region of the homodimer. The expectation was that the presence of an intact disulphide in the stalk might rigidify the stalk, making the overall structure less compact. Two complexes formed with the monomer and two different Fabs (5.11A1 and 9D7) gave crystals, but only one of these crystal forms (obtained with 5.11A1 Fab fragments) proved to be suitable for data collection. Other antibodies may also have been useful in crystallising CD28, including antibodies that bind to the same loop of CD28 as bound by 5.11A1 (the C'-D loop) or that bind to the ligand binding site of CD28. Suitable antibodies are described in US-A1-2003/0166860 and Luhder et al (2003) J. Exp. Med., 197, 955-66.

Preparation of CD28 homodimer

(i) Construct generation

The polymerase chain reaction (PCR) was used to amplify complementary DNA (cDNA) encoding the signal peptide sequence of mouse immunoglobulin heavy chain and the extracellular domain of CD28 (residues 1-134 of the mature polypeptide; SEQ ID NO:1) from 44 ng of the plasmid, pKGe1145. The oligonucleotides used in the reaction added, at the 5' end, an Xba I cleavage site and 24 nt of the rat CD4 5' untranslated region and, at the 3' end, codons for the thrombin cleavage site, LVPRGS. The sequences of the oligonucleotide primers used for this were (oligonucleotide sequences are given in 5' to 3' direction) CD28T_5': TAG TAG TCT AGA CCC CAT CCG CTC AAG CAG GCC ACC ATG GAT TGG CTG CGG AAC TTG; and CD28T 3': CTA CCA CTA CCC CTG GGT ACC AGG GGC TTA G. In a second reaction, cDNA encoding the heavy chain constant (C) region-2 and C region-3 domains of murine Ig (residues 103-323 of the secreted protein) was amplified by PCR from 44 ng of pKGe1145. At the 3' end, the oligonucleotides added an Xba I restriction site to aid cloning. The NH2-terminus of the protein encoded by the Ig cDNA had the sequence GSKPSIS rather than GCKPCIC. The sequences of the oligonucleotide primers for this reaction were Ig_5': CTA AGC CCC TGG TAC CCA GGG GTA GTG

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GTA G; and Ig_3': CTA CTA TCT AGA TTA TTT ACC AGG AGA GTG GGA G. The PCR conditions for both reactions were: denaturation at 94°C for 15s, annealing at 59°C for 30s, extension at 68°C for 210s; 2.5U of Accuzyme polymerase (Bioline Ltd, U.K.), 300 nM oligonucleotides and 200 µM dNTPs were used and the reactions run for 20 cycles.

In a third reaction, PCR was used to anneal the two initial products together to generate cDNA encoding a chimera consisting of the CD28 extracellular domain fused to murine IgGFc via a thrombin cleavable sequence (called the CD28TFc chimera; SEQ ID NO:2). Ten microlitres of each of the initial PCR reaction product mixtures was used as template and 300 nM of the CD28_5' and Ig_3' oligonucleotides was also added to the mix. The PCR conditions were otherwise identical to the first set except that they were run for only 4 cycles. The PCR product was gel-purified, cut with Xba I and cloned into the Xba I site of pEE14 for expression in the glutamine synthetase-based gene expression system (Łonza Biologics Plc, UK). The plasmid construct was then sequenced using dideoxy sequencing.

(ii) Expression of the CD28TFc chimera

Lec3.2.8.1 cells, 2 x 10⁶/flask, were transfected with 20 μg of DNA/flask for 3h using Pfx-8 lipids (Invitrogen Inc), and then the cells were cloned the following day by plating out at 2 x 10⁶ cells/96-well plate. After 2 weeks, the clones expressing the highest amounts of CD28TFc were selected by Western-blotting using the semi-quantitive ECL detection system (Amersham-Pharmacia, UK) and an anti-mouse Fc primary antibody (Sigma-Aldrich Co.). The best-expressing clone was expanded and grown to confluence in bulk culture in Cell Factories (Nunc A/S, Denmark) containing immunoglobulin-free medium (Invitrogen-Gibco Ltd, UK) in the presence of 2mM sodium butyrate. The supernatant was harvested after approximately four weeks and clarified by centrifugation at 5,000g.

(iii) CD28TFc purification

The spent, clarified medium was concentrated to approximately 1/6 of the original volume using a Masterflex L/S concentrator (Helixx Technologies, Inc.). The sample was then buffer-exchanged against the original volume of 3M NaCl, 1.5M

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glycine, pH 8.5 high-salt buffer and the protein incubated with Protein A Sepharose beads (Sigma-Aldrich Co.) using 10 mls of swollen beads/litre of concentrated supernatant at 1 litre of supernatant/5 litre conical flask or beaker. The pH was adjusted to pH 8.5 with 2.75 M Tris, pH 8.5 to allow binding of the CD28TFc to Protein A overnight with gentle stirring at 4°C.

The beads were allowed to settle for 2 h prior to siphoning off the depleted supernatant. The settled beads were then transferred to 50 ml Falcon tubes (Becton Dickinson Biosciences, UK) and recovered by centrifugation at 200g. The beads were transferred to a 30 ml column (Biorad, UK) and then washed with 300 mls of cold phosphate-buffered saline, 0.5 M NaCl, pH 8.3. The column was eluted with 0.1 M citric acid, pH 3.0 into 10 x 2 ml fractions in glass tubes containing 0.4 ml of 2.75M Tris, pH 8.5 for immediate neutralization of the citric acid. Fractions containing CD28TFc according to analysis by 12% sodium dodecyl sulphate polyacrylamide gel electrophoresis (SDS-PAGE) were concentrated to 0.5ml or no higher concentration than 20 mg/ml using a Centriprep 10 concentrator (Millipore Corp). The protein was then applied to a Superdex 200 H/R gel filtration column (Amersham Biosciences) preequilibrated with 10 mM Hepes, 140 mM NaCl, pH 7.4 (HBS buffer) for up to three successive runs. Eluting fractions were monitored for absorbance at 280 nm. Proteincontaining fractions were examined by SDS-PAGE. Each cycle of batch purification yielded ~9 mgs of CD28TFc; up to 7 batch-purfications was required to deplete all the CD28TFc per set of 6 cell factories (~5 litres of starting tissue culture supernatant).

(iv) Thrombin protease cleavage of CD28TFc

The most-pure fractions containing CD28TFc were pooled for thrombin cleavage. Initial trial titrations dictated the use of the following conditions for large-scale cleavage of CD2TFc: lyophilized thrombin (Sigma-Aldrich Co.) was re-hydrated in HBS buffer to a concentration of 1U/µl and this was then added to the CD28TFc at 0.11 µl/6 µg of protein for overnight digestion at 37°C. The reaction was stopped by addition of freshly re-hydrated benzamidine to a final concentration of 1mM. A 12% non-reducing SDS-PAGE gel was used to confirm the extent of cleavage.

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(v) Purification of the CD28 homodimer

The pH of the thrombin-cleaved protein was adjusted to pH 8.5 using 2.75M Tris pH 8.5, prior to concentration to 0.5 ml using a Centriprep 10 concentrator (Millipore Corp). Fresh Protein A beads were washed and rehydrated to a final volume of ~5 mls, prior to being packed into a 0.7 cm x 20 cm Econo-column (Bio-Rad, U.K.) and then equilibriated with HBS, pH 8.5 at 4°C. The concentrated protein was then applied to the column, allowed to run into the bed, and then sequential fractions were eluted by addition of 0.5 ml of HBS, pH 8.5 to the top of the bed every 10 minutes for 2h. The absorbance of each fraction was determined at 280 nm. The extent of separation of the Fc from the thrombin-released CD28 homodimer was determined by 12% SDS-PAGE analysis of the fractions under non-reducing conditions. The critical steps for good separation were (1) to allow the protein to pass slowly through the column and (2) to conduct the separation at 4°C. The homodimer was concentrated to 0.5 ml and subjected to gel-filtration on a Superdex 75 H/R column (Amersham Biosciences). The purified homodimer was used for crystallization trials, reduced and alkylated for other crystallization trials (see below), or frozen at -80°C for future use.

Preparation of Fab fragments of 5.11A1 antibody

Fab fragments were prepared using the Pierce Biotechnology ImmunoPure® Fab Preparation Kit, as briefly outlined below.

(i) Fab fragment generation and purification

Nine millilitres of whole, purified 5.11A1 antibody at 0.3 mg/ml in PBS was concentrated to 1 ml and then diluted to 10 mls with 20 mM sodium phosphate, 10 mM EDTA, pH 7 and then re-concentrated to 0.5 ml. To this was added 0.5 ml of 20 mM sodium phosphate, pH 7 containing 3.5 mg/ml cysteine•HCl. The 1 ml mixture was then added to 0.5 ml of a 50% slurry of Sepharose-immobilized Papain supplied with the kit, which had been pre-equilibrated with 20 mM sodium phosphate pH 7 containing 3.5 mg/ml cysteine•HCl. This was then incubated for 5 hours in a shaking water bath at 37°C. The cleaved Fab and Fc fragments and undigested IgG were separated from the Immobilized Papain beads by centrifugation at 1000g and the beads rinsed with 1.5 ml of the ImmunoPure IgG Binding Buffer supplied with the kit. The wash was then combined with the crude digest and the mix applied to a Sepharose-immobilized Protein

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A column pre-equilibrated with 13 ml of ImmunoPure IgG Binding Buffer. The column was washed with 6.0 ml of the Binding Buffer and the eluate containing the Fab fragments collected (9 mls in total). The eluate was concentrated to 0.5 ml and applied to a Superdex 200 H/R gel filtration column (Amersham Biosciences) pre-equilibrated with HBS buffer. Eluting fractions were monitored for absorbance at 280 nm. Protein-containing fractions were examined by SDS-PAGE.

Preparation of a crystallizable form of CD28

(i) Reduction and alkylation of CD28

CD28 has an interchain disulphide bond within the "stalk-like" region that is largely responsible for homodimerization. It was speculated that its location within the stalk would render it more sensitive to reducing agents than the "canonical" disulphide bond and one other disulphide buried within the ligand-binding domain. If true this meant that monomeric CD28 could be generated which was native-like and fully active for ligand and antibody binding. The minimum concentration of reducing agent required to release the monomer was ascertained by titrating the reducing agent, dithiothreitol (DTT). The reduced cysteines in the protein and excess DTT were each then inactivated by alkylation with a 2.2-fold molar excess of iodoacetamide (IAA). This titration indicated that the optimal conditions were 12.5 µM protein, 1.5mM DTT and 3.3 mM IAA. The reduced protein sample, generally ~4 ml, was finally concentrated to 0.5 ml and separated from unreduced homodimer by gel-filtration on a Superdex 75 H/R column (Amersham Biosciences).

Crystallographic methods

(i) Crystallization and data collection

The CD28/5.11A1 Fab complex was formed by incubating a 2:1 molar ratio of CD28 and Fab, followed by concentration of the protein mixture to 15.6 mg/ml in HBS (the extinction coefficient, ε , of CD28 is 1.7 and that of the Fab is 1.4). Crystals were grown at 18°C in 0.2 μ l hanging drops (0.1 μ l of the protein mixture plus 0.1 μ l of precipitating reagent) set up using a Cartesian Robot (APS Robotics & Integration, Ilc; Brown et al (2003) J. Appl. Cryst. 36, 315-18). The precipitating reagent consisted of a mixture of 0.2 M magnesium formate and 20% polyethylene glycol 3350 in water.

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Crystals appeared in 5-7 days and were cooled to 100K in the precipitating reagent with glycerol added to a final concentration of 10%, using a Cryojet liquid nitrogen system for data collection (Oxford Instruments, Abingdon, UK). Crystals belong to space group C2 with unit cell dimensions a = 191.2, b = 47.4, c = 71.8 Å and a calculated solvent content of 56-58% for one CD28 monomer and one Fab molecule per asymmetric unit (ignoring the effects of glycosylation). The 2.7Å resolution data were collected from a single crystal at 100K at Beamline ID2 at the European Synchrotron Radiation Facility using a FReLoN CCD. One hundred and fifty-eight 1° rotation images were collected and reduced with HKL2000 (Otwinowski and Minor (1997) Methods Enzym. 276, 307-26).

(ii) Structure determination and refinement

The structure was solved by molecular replacement in XPLOR v3.851 (Brünger (1992) X-PLOR Version 3.1. A system for X-ray crystallography and NMR. Yale University Press, New Haven, CT.) using a set of search models generated from a single Fab structure (PDB accession no. 15c8) by varying the elbow angle in 2° steps using an XPLOR script. A single unambiguous solution was found when the elbow angle was altered by -8° as defined by the script. After rigid body refinement of each domain of the Fab in CNS (Brünger et al. (1998) Acta Cryst. D54, 905-21), the R-factor was 44.4%. Initial electron density maps phased with Fab alone showed very limited, if any, electron density for the CD28 molecule. The Fab model was mutated to the sequence of 5.11A1 before proceeding with two cycles of manual rebuilding in O (Jones et al (1990) O: A macromolecular modelling environment. Crystallographic and modeling methods in molecular design. Bugg and Ealick, Eds. Springer-Verlag Press 189-95) and positional refinement in CNS, reducing the R-factor to 36.4%. A molecular replacement solution for CD28 was then found by using only regions of human CTLA-4 (from PDB 1i8l) with strong sequence homology to CD28, i.e. all the β-strands (except C') and the EF and FG loops, as a search model and by fixing the refined Fab structure. In order to avoid model bias, the refined constant regions of the Fab were replaced with the unaltered constant domains from PDB 15c8 by superposition using SHP (Stuart et al (1979) J. Mol. Biol. 134, 109-42), and the positions were fixed during refinement. The variable regions of the Fab and the CD28 monomer were refined in X-PLOR v3.851

using positional refinement followed by grouped and restrained individual B factor refinement along with manual rebuilding in O. All refinement procedures used data from 25.0-2.7Å and excluded 5% of reflections randomly selected for generation of the R_{free} data set. The anisotropy of the data was corrected for using X-PLOR and the data were sharpened for all but the last round of refinement. The current model has an R factor of 25.3% and an R_{free} of 33.4% against all data to 2.7Å. The model includes the CD28 monomer (excluding its C-terminal stalk) from residues 2 to 118, excluding residues Leu28 and Phe29, which are poorly ordered, and the Fab, but with none of the sugar chains built onto the CD28. The model has 76% of residues in the most favoured regions of the Ramachandran plot, with a further 21% in additionally allowed regions.

The structure of a CD28-superagonist antibody complex

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The ligand-binding V-set IgSF domain of the CD28 monomer, solved in complex with 5.11A1 Fab, is very similar to the equivalent region of CTLA-4. Lattice contacts generate a plausible CD28 homodimer. Whilst this dimer is similar to the CTLA-4 homodimer (which is bivalent), the arrangement of the monomers in CD28 is sufficiently distinct to suggest an explanation for the apparent monovalence of CD28, i.e. the membrane proximal domains of ligands competing for each ligand binding site are likely to clash. Cryoelectron microscopic analyses show that both classes of antibodies are bivalent, ruling out aggregation-based explanations for the differential signalling effects of conventional versus superagonistic antibodies. The 5.11A1 Fab fragment binds orthogonally to the surface formed by the CC'C" strands of CD28, favouring the C'C" "edge" of the monomer. This places the two long axes of the Fabs parallel to each other and the cell surface. In contrast, the epitopes of the conventional antibodies are close to the ligand binding "top" of the homodimer.

Signalling by receptors dependent on extrinsic kinases

The existence of two classes of activating anti-CD28 antibodies, i.e. costimulatory antibodies and superagonists, greatly simplifies the analysis of signalling by this archetypal costimulatory receptor. The observation that the two antibody classes have homologous effects in two different species, and that these effects are predictable simply according to the location of their epitopes, rules out

trivial explanations for the distinct signalling properties of these antibodies, e.g. affinity differences. Instead, the receptor-triggering problem is reduced to a comparison of the structural properties of the complexes that these two types of antibodies form with CD28.

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From the present crystal structure of the complex of CD28 with a superagonistic antibody, it can be deduced that an antibody-induced increase in the net phosphorylation of the cytoplasmic domain of a given cell surface receptor, due to changes in the rates of phosphorylation and dephosphorylation of it, results in the triggering of that receptor (see Figure 1). In more detail, the antibodies hold the cell surface at certain distances from an immobilizing substrate (i.e. other, Fc receptorbearing cells, in vivo or plastic, in vitro), such that the membrane separation in the region of the immobilized antibody and receptor will differentially exclude, from the immediate vicinity of the receptor, other molecules whose extracellular domains are comparable in size or larger than CD28-antibody complexes, such as the tyrosine phosphatase, CD45. In contrast, tyrosine kinases, e.g. p56lck, will be unaffected because they are small and/or attached to the inner leaflet of the membrane. The result is that, overall, the phosphorylation of CD28 will be favoured over its dephoshorylation (by CD45), with the net increase in phosphorylation amounting to receptor triggering. Superagonists are more potent than conventional antibodies because they bind epitopes close to the membrane rather than at the "top" of the molecule, leading to more efficient segregation of, e.g. CD45, and therefore a larger increase in the net phosphorylation of CD28.

The important corollary of this explanation is that antibodies that bind the membrane-proximal epitopes of the large number of other cell surface molecules not belonging to the CD28 subset of the immunoglobulin superfamily, but sharing the key signalling property of CD28-subset molecules, *i.e.* a reliance on extrinsic tyrosine kinases, for example PD-1 and BTLA, should also potently invoke the activating or inhibitory signalling properties of those molecules in precisely the same way, allowing the manipulation of cell behaviour with such antibodies.

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PD-1 and BTLA

Programmed Death (PD)-1 protein modulates the responses of previously activated T- and B-cells in secondary lymphoid organs or peripheral (parenchymal) tissues. PD-1 is expressed on a subset of thymocytes and upregulated on activated T, B and myeloid cells. The PD-1 ligands, B7-H1 and B7-DC, are more widely expressed than those of CD28 family members and are induced by pro-inflammatory agents on monocytes and dendritic cells and on activated but not resting B cells. B7-DC is expressed in a variety of peripheral tissues, including heart, pancreas, lung and liver. The B and T lymphocyte attenuator (BTLA), is also expressed on activated T and B cells, but attenuates production of IL-2 after binding a different peripherally expressed B7-related protein, called B7x.

PD-1 and BTLA are structurally comparable to other members of the CD28 family only insofar as the proteins also consist of a single V-set IgSF domain supported on stalks, and the cytoplasmic domains contain immunoreceptor tyrosine-based motifs (inhibitory in these two cases). The sequences of the IgSF domains of PD-1 and BTLA indicate that these proteins are unrelated and *do not* belong to the same subset of the IgSF as CD28. Consistent with the view that PD-1 is involved in maintaining tolerance in normal T cells in the periphery, mice lacking the gene develop a variety of autoimmune-like diseases dependent on the genetic background, including lupus-like arthritis and glomerulonephritis, and have increased serum IgG3 and augmented B-cell proliferative responses to anti-IgM *in vivo*.

Activating signalling by PD-1 and BTLA, because these molecules are inhibitory, would be expected to dampen a variety of peripheral immune pathologies. Signalling of this type could be stimulated by the binding of superagonistic antibodies to the membrane proximal regions of these proteins. A set of additional molecules, each of which has inhibitory immunoreceptor tyrosine-based signalling motifs and are therefore targets for generating superagonists, is shown in Table 2.

Identifying epitopes for superagonists

The procedure is as follows. The "lower", membrane-proximal half of the membrane proximal domain of a given structure, e.g. CD28 in Figure 2A, is identified by visual inspection of the structure. Superagonistic agents bind residues in

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this region. For identifying superagonistic agents in receptors closely related to the known structure, the equivalent regions are identified in an alignment of the sequence of the known structure with that of the related proteins as shown in Figure 2A. To identify the epitopes of superagonistic antibodies in other molecules that have the requisite signalling properties but for which there is no structure, e.g. PD-1 in Figure 2B, a structural model is identified by alignment of the sequence with that of the most similar molecule of known structure in the Protein Data Bank (in the example in Figure 2B, the variable domain of the Ig kappa chain is the structure with the most similar sequence to PD-1). The "lower", membrane proximal half of this domain is highlighted on the structure by visual inspection and the equivalent regions are identified in the sequence alignment. To screen for superagonists, the second and third residues "down" (i.e. toward the membrane) in the marked epitopes shown in parts A and B are identified as shown in Figures 2C and 2D. These residues, singly or together preferably form at least part of the epitopes of antibodies or other superagonistic agents, as binding to these residues will require that the binding of the agent is parallel with the cell membrane. These residues can therefore be mutated in proteins used for screening the superagonistic agents (i.e. agents binding to the unmutated protein but not the mutated protein, should be superagonistic).

Table 1

CD28 family superagonistic epitopes

Epitopes are named according to the strands from which they derive.

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	Ð	NGTIIHV	NGTQIYV	TGGYLHI	
	F	TDIYFC	TGLYIC	ANYYFC	
	E	FYLQN	LTIQG	FFLYN	
	$C_{"}D$	VYSKTGFNCDG	FLDDSICTG	VSIKSLKFCHS	
-	C-C′	SLHKGLDSAVEVCV	TVLRQADSQVTEVCA	QLIKGGOILCD	
	B	AVNLS	GIASFV	GVQIL	
	A'	SPMLV	PAVVL	YEMFI	
	Protein	hCD28	hCTLA-4	PICOS	

PD-1 and BTLA superagonistic epitopès

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Protein	A	В	C-C	C"- D	E	F	Ð
hPD-1	PALLVV	DNATF	RMSPSNQTDK	QPGQDCRFR	MSVVR	NDSGTY	LRAELR
hBTLA	QSEHSI	DPFEL	KLNG	QTSWK	LHFEP	NDNGSY	TTLYVT

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Table 3

Sequence	GNYSQQLQVYSKTGF	YMMGNELTFLDDS	KTKGSGNTVSIKSLK	LAAFPEDRSQPGQDCR
Protein	hCD28	hCTLA-4	HCOS	hPD-1

Table 2

Targets of inhibitory superagonist antibodies

Receptor	Chromosome	Expression	no. of ITIMs
FcRIIB	1q23-24	B, myeloid, mast	1
PILR	7q22	Myeloid	2
CD72	9p	\mathbf{B}^{-}	2
CD5	11q13	T, subset B	1
MAFA	12p12-13	Myeloid, mast, NK	1 .
NKG2A	12p13.1-13.2	NK, T	2
CD31	17q23	Myeloid, etc	1
CMRF35H	17q24	Leukocytes	3
CD22	19q13.1	В	4
CD66a	19q13.2	Granulocytes, etc	2
CD66d	19q13.2	Granulocytes	1
CD33	19q13.3	Myeloid	1
SIGLEC5	19q13.3	Myeloid	1
SIGLEC6	19q13.3	B cells, myeloid	1
SIGLEC7	19q13.3	NK, myeloid, etc	1
ILT2,3,4,5	19q13.4	Myeloid, B, etc	4
LIR8	19q13.4	Myeloid, B, etc	4
LAIR-1	19q13.4	Leukocytes	2
KIR2DL	19q13.4	NK, T	2
KIR3DL	19q13.4	NK, T	2
SIRP	20p13	Myeloid, etc	2

Table 4
Co-ordinates of the CD28/5.11A1 crystal structure

REMARK FILENAME="/mnt/safe6/ed/cd28/cd28_all/xplor/ref18/positionaln3.pdb" R= 0.251035 from 25 to 2.7 REMARK created by user: robert 09:48:19 REMARK DATE: 09-Jan-04 L 122.280 49.781 38.327 1.00 64.18 ASP 1 CBATOM 1 L 1.00 67.78 123.319 49.071 37.463 ATOM CG ASP 1 2 1.00 66.82 L 36.470 122.934 48.417 OD1 ASP 1 MOTA 1.00 54.04 L 124.524 37.779 49.162 1, OD2 ASP 4 ATOM L 1.00 50.51 52.265 38.005 122.104 1 C ASP ATOM 5 \mathbf{L} 1.00 41.52 53.057 37.163 122.541 б ASP 1 0 ATOM L 1.00 37.53 121.674 36.112 50.711 1 ASP 7 \mathbf{N} MOTA L 1.00 50.29 37.579 50.905 121.547 ASP CA 8 MOTA L 39.314 1.00 51.24 52.527 122.073 ILE N2 9 MOTA L 1.00 50.84 39.890 122.567 53.783 2 ILE CA MOTA 10 L 1.00 22.62 41.240 121.842 54.094 2 11 CBILE MOTA 1.00 18.55 \mathbb{L} 41.781 55.454 122.278 CG2 ILE 2 12 MOTA 41.022 L 1.00 30.61 54.081 120.327 2 13 CG1 ILE MOTA 42.229 L 1.00 31.86 2 54.521 119.510 14 CD1 ILE MOTA 1.00 54.91 \mathbb{L} 40.119 53.714 2 124.086 15 ILE C MOTA 1.00 55.68 L 40.283 124.645 52.630 2 16 , 0 ILE MOTA 40.136 1.00 58.93 L 124.749 54.869 3 17 GLNMOTA \mathbf{N} 1.00 56.95 L 40.322 54.923 126.204 GLN 18 CA 3 ATOM L 1.00 60.02 39.145 55.679 126.847 3 GLN19 CB MOTA 1.00 63.51 L 37.863 54.851 127.010 GLN3 20 CG MOTA L 1.00 65.36 55.552 36.615 126.479 GLNCD 3 21 ATOM 1.00 62.07 Ŀ 36.174 127.024 56.568 3 OE1 GLN 22 ATOM 1.00 72.37 L 125.412 36.038 55.003 GLN 3 23 NE2 MOTA 1.00 51.69 41.650 L 55.564 126.635 3 C GLN ATOM 24 42.004 1.00 54.63 \mathbb{L} 126.179 56.649 3 25 0 GLN MOTA Ŀ 42.376 1.00 42.42 54.889 127.522 MET 4 26 \mathbf{N} MOTA 1.00 37.64 43.660 L 128.005 55.392 MOTA 27 CA MET -4 1.00 54.55 L 54.248 44.671 128.066 MET CB 28 4 MOTA 1.00 56.74 \mathbf{L} 45.783 127.037 54.319 CG MET MOTA 29 4 L 1.00 76.06 45.189 54.633 125.360 MET 4 30 MOTA SD Ţ 1.00 68.01 56.269 45.843 MET 125.083 4 MOTA CE 31 \mathbf{L} 1.00 44.16 43.507 129.392 56.008 32 MET MOTA C 4 1.00 35.72 L 43.176 55.311 130.358 MET 4 MOTA 33 0 43.750 57.310 1.00 50.40 卫 5 129.496 34 ASN MOTA NL 1.00 58.90 43.624 57.996 130.779 5 ASN MOTA 35 CA \mathbf{L} 1.00 67.94 59.060 42.521 5 130.703 ASN MOTA 36 CB 1.00 59.91 L 41.233 58.517 130.113 5 37 CG ASN MOTA L 40.474 57.811 1.00 49.08 130.783 5 OD1 ASN 38 MOTA L 1.00 56.43 58.839 40.981 128.848 ND2 ASN 5 MOTA 39 1.00 46.55 L 58.643 44.939 131.191 40 ASN 5 MOTA C 1.00 40.94 \mathbf{L} 59.637 45.368 130.612 ASN 5 0 MOTA 41 L 1.00 33.77 58.076 45.577 132.202 GLNб \mathbf{N} MOTA 42 1.00 36.85 \mathbf{L} 46.846 132.661 58.607 б GLN43 CA MOTA 1.00 24.74 L 57.476 47.679 133.257 GLN6 CB ATOM 44 1.00 19.84 L 56.218 47.684 132.395 45 CG GLN 6 MOTA 1.00 27.56 L 132.393 55.524 49.029 GLN6 46 ATOM CD

(m)							•	•	ž n			
ATOM	47	OE1	GLN	√ ¹ 6		132.925	56.048	50.013	1.00	30.84		L
ATOM	48	NE2	GLN	· 6		131.803	54.339	49.082	1.00	34.41	•	L
ATOM	49	C	GLN	6	1	133.677	59.725	46.647	1.00	43.10	,,	L
MOTA	50	0	GLN	6		134.328	59.800	45.608	1.00	55.89		L
MOTA	51	N	SER	7		133.807	60.598	47.641	1.00	47.45	-	L
MOTA	52	CA	SER	. 7		134.736	61.714	47.543	1.00 !	54.98		·L
ATOM	53	CB	SER	7		134.285	62.858	48.469	1.00	70.71	•	Ŀ
ATOM	54	OG	SER	7		135.232	63.917	48.514	1.00	51.37		L
ATOM	55	C	SER	7		136.187	61.304	47.812	1.00 !	57.75		L
ATOM	56	0	SER	7	r	136.828	60.732	46.928	1.00	58.97		L,
ATOM	57	N	PRO	8		136.722	61.540	49.029	1.00 4	48.65		L
ATOM	58	CD	PRO	8	ŧ	136.250	62.116	50.300	1.00	21.82		Ļ
ATOM	59	CA	PRO	8		138.118	61.109	49.140	1.00 4	47.63		L
ATOM	60	CB	PRO	, 8		138.515	61.533	50.559	1.00	29.91		L
ATOM	61	CG	PRO	8		137.525	62.576	50.933	1.00 2	26.41		L
ATOM	62	C	PRO	8		138.358	59.622	48.893	1.00 4	18.77		Lı
ATOM	63	0	PRO	8		137.820	58.772	49.604	1.00 6	53.86		L
ATOM	64	N	SER	9		139.161	59.318	47.876	1.00	33.02		L
ATOM	65	CA	SER	9		139.500	57.939	47.548	1.00	32.48		L
ATOM	66	CB	SER	9		140.151	57.864	46.169	1.00 3	30.85		L
ATOM	67	OG	SER	9		141.554	57.812	46.286	1.00 2	25.75		L
ATOM	68	C	SER	9		140.469	57.407	48.602	1.00 3	30.90		L
ATOM	69	0	SER	· 9	,	140.661	56.197	48.737	1.00 3	32.96		L
ATOM	70	N	SER	10	j.	141.076	58.333	49.340	1.00 2	29.68		L
ATOM	71	CA	SER	. 10		142.022	58.018	50.412	1.00 3	35.34		L
ATOM ·	72	CB	SER	10		143.387	57.645	49.831	1.00 4	19.82		L
ATOM	73	OG	SER	10		144.392	58.538	50.289	1.00 8	31.38	"	L
ATOM	74	C	SER	·. 10		142.161	59.254	51.308	1.00 3	31.04		L
ATOM.	75	0	SER	10		141.964	60.379	50.839	1.00 3	35.88	,	L
ATOM	76	И.	LEU	. 11		142.502	59.056	52.582	1.00 2	27.16		Li
ATOM	77	CA	LEU	11		142.634	60.181	53.498	1.00 2	24.50		Ŀ
ATOM	78	CB	LEU	11		141.258	60.780	53.780	1.00 4	17.56		L
MOTA	79	CG	LEU	11		141.120	61.488	55.134	1.00 5	57.17	:	Lı
MOTA	80	CD1	LEU	11		141.752	62.878	55.063	1.00 6	55.58	,	L
ATOM	.81	CD2	LEU	-11		139.650	61.583	55.509	1.00 6	51.17		L
MOTA	82	C ,	LEU	11		143.308	59.884	54.831	1.00 2	22.63	**	Ŀ
ATOM	83	0	LEU	11		142.978	58.919	55.508	1.00 2	25.60		L
MOTA	84	N	SER	12		144.233	60.759	55.209	1.00	33.11		L
ATOM	85	CA	SER	12		144.965	60.653	56.466	1.00 3	35.62		L
ATOM	86	CB	SER	12	•	146.465	60.745	56.201	1.00 3	34.92		L ¯
ATOM	87	OG	SER	12		147.186	60.895	57.409	1.00 2	29.53		Ľ,
MOTA	88	C	SER	12		144.534	61.798	57.392	1.00 3	38.38	ı	L
MOTA	89	0	SER	12		144.226	62.894	56.928	1.00 4	46.48		L
ATOM	90	N	ALA.	13		144.519	61.546	.58.696	1.00 3	31.39	i	L
ATOM	91	CA	ALA	13		144.116	62.559	59.666	1.00 3	34.62	•	L
MOTA	92	CB	ALA	13		142.615	62.610	59.753	1.00 2	28.98		L
ATOM	93	C	ALA	13		144.706	62.178	61.012	1.00 3	88.12	•	L
MOTA	94	0	ALA	13		144.928	61.002	61.268	1.00 4	11.17	÷	L
MOTA	95	N	SER	14		144.946	63.156	61.878	1.00 3	36.11	"	L
MOTA	96	CA	SER	14		145.553	62.865	63.177	1.00 4	2.50		L
MOTA	97	CB	SER	14		146.477	64.012	63.593	.1.00 4	5.35		L
ATOM	98	QG	SER	14		147.608	63.522	64.299	1.00 5	51.37		L
ATOM	99	C	SER	14		144.618	62.553	64.343	1.00 3	86.84		L

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ATOM	100	0	SER	14	143.395	62.586	64.217	1.00 30.77	L
ATOM	101	N	LEU	15	145.246	62.246	65.477	1.00 42.69	\mathbf{L}_{i}
MOTA	102	CA	LEU	15	144.588	61.919	66.737	1.00 51.12	L
ATOM	103	CB	LEU	- 15	145.077	62.874	67.829	1.00 35.76	L
ATOM	104	CG	LEU	15	145.549	64.244	67.331	1.00 50.27	L
ATOM	105	CD1	LEU	.15	144.709	65.353	67.956	1.00 45.12	$\mathbf{L}_{\mathbf{l}}$
ATOM	106	CD2	LEU	15	147.023	64.425	67.671	1.00 46.79	L
ATOM	107	C	LEU	15	143.071	61.968	66.666	1.00 63.00	L
ATOM	108	0	LEU	15	142.440	61.062	66.125	1.00 71.25	\mathbf{L}
ATOM	109	N	GLY	16	142.495	63.029	67.229	1.00 61.62	L
ATOM	110	CA	GLY	16	141.052	63.182	67.225	1.00 58.47	L
ATOM	111	C	GLY ·	16	140.588	64.176	66.177	1.00 62.05	, · L
ATOM	112	0	GLY	16	139.827	65.094	66.481	1.00 59.73	$\mathbf{L}_{\mathbf{i}}$
ATOM	113	N	ASP	17	141.052	63.991	64.942	1.00 62.73	Ŀ
ATOM	114	CA	ASP	17	140.690	64.863	63.828	1.00 55.42	L
ATOM	115	CB	ASP	17	141.729	64.728	62.715	1.00 45.39	${f L}$
MOTA	116	CG	ASP	17	142.006	66.039	62.017	1.00 56.02	Ŀ
ATOM	117	OD1	ASP	17	142.467	66.992	62.682	1.00 51.84	L
ATOM	118	OD2		17	141.762	66.116	60.795	1.00 64.45	L
ATOM	119	C	ASP	17	139.313	64.470	63.298	1.00 54.85	L
ATOM	120	0.	ASP	17	139.066	63.296	63.027	1.00 69.38	${f L}$
ATOM	121	N	THR	18	138.425	65.448	63.150	1.00 39.55	L
ATOM	122	CA	THR	18	137.073	65.189	62.661	1.00 35.18	Ļ
ATOM	123	CB	THR	18	136.089	66.238	63.211	1.00 39.72	L
ATOM	124	OG1	THR	18	136.155	66.250	64.644	1.00 36.21	L
ATOM	125	CG2	THR	18	134.668	65.918	62.774	1.00 28.85	L
ATOM	126	C	THR	18	136.967	65.172	61.132	1.00 39.85	L
ATOM	127	0	THR	18	136.590	66.167	60.522	1.00 51.97	L
ATOM	128	N	ILE	19	137.289	64.035	60.521	1.00 38.56	L
ATOM	129	CA	ILE	19	137.233	63.881	59.065	1.00 40.49	Ľ
ATOM	130	CB	ILE	19	137.917	.62.579	58.621	1.00 43.22	L
ATOM	131	CG2	ILE	19	139.334	62.545	59.144	1.00 53.54	L
ATOM	132	CG1	ILE	19	137.148	61.373	59.161	1.00 31.99	· L
ATOM ·	133	CD1	ILE	19	136.020	60.889	58.260	1.00 27.22	· L
ATOM	134	C	ILE	19	135.811	63.857	58.519	1.00 41.63	L
ATOM	135	0 -	ILE	19	134.850	63.825	59.284	1.00 48.28	L
ATOM	136	N	THR	20	135.690	63.839	57.191	1.00 41.74	L
ATOM	137	CA	THR	20	134.388	63.814	56.517	1.00 46.28	L
ATOM	138	CB	THR	20	133.761	65.246	56.473	1.00 55.85	L
ATOM	139	OG1		20	132.666	65.316	57.396	1.00 68.15	L
ATOM	140	CG2	THR	20	133.260	65.592	55.073	1.00 57.90	Ŀ
ATOM	141	C	THR	20	134.516	63.260	55.090	1.00 34.62	L
ATOM	142	0 .	THR	20	135.433	63.620	54.351	1.00 35.05	L
ATOM	143	N	ILE	.21	133.592	62.385	54.706	1.00 27.66	L
ATOM	144	CA	ILE	21	133.613	61.793	53.371	1.00 40.68	L
ATOM	145	CB	ILE	21	133.646	60.260	53.466	1.00 45.17	L
ATOM	146	CG2	ILE	21	133.946	59.641	52.110	1.00 58.28	Ŀ
ATOM	147	CG1	ILE	21	134.757		54.432	1.00 37.17	L
ATOM	148	CD1	ILE	21	134.556	58.489	55.038	1.00 30.25	L
ATOM	149	G CD ^T	ILE	21	132.412	62.266	52.552	1.00 41.14	L
ATOM	150	0	ILE	21	131.706	63.173	52.978	1.00 52.31	L T
		N	THR	22	132.176	61.669	51.386	1.00 37.16	L
ATOM	151 152			22	131.069	62.096	50.533	1.00 37.13	L
MOTA	152	CA	THR	44	TOT.002	02.090	20.000	1.00 J0.J1	

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ATOM	15:	3 CB	THR	22	131.426	63.392	49.791	1.00 33.17	L
ATOM	*	4 OG1	THR	22	131.754	64.417	50.736	1.00 20.87	\mathbf{L}
ATOM			THR	22	130.270	63.832	48.913	1.00 26.45	L
ATOM		•	THR	22	130.703	61.078	49.462	1.00 45.82	L
ATOM			THR	22	131.563	60.656	48.694	1.00 54.24	${f L}$
ATOM			CYS	23	129.430	60.705	49.381	1.00 50.07	L
ATOM			CYS	23	129.004	59.746	48.363	1.00 63.67	L
ATOM			CYS	23	127.790	60.230	47.570	1.00 68.93	L
ATOM			CYS	23	126.651	60.017	47.983	1.00 85.32	L
ATOM			CYS	23	128.682	58.384	48.998	1.00 53.28	L
ATOM			CYS	23	127.931	57.193	47.829	1.00 60.78	L
ATOM			HIS	24	128.035	60.874	46.432	1.00 62.30	${f L}$
ATOM			HIS	24	126.958	61.376	45.581	1.00 55.79	L
ATOM			HIS	24	127.438	62.585	44.766	1.00 66.11	L
ATOM			HIS	24	127.210	63.903	45.443	1.00 94.47	· L
ATOM	•			24	127.360	64.280	46.736	1.00100.00	L
ATOM				24	126.760	65.020	44.771	1.00 99.99	L
				24	126.647	66.029	45.618	1.00 96.64	L
ATOM ATOM				24	127.005	65.605	46.818	1.00100.00	L
-	1	1	HIS	24	126.456	60.282	44.636	1.00 53.07	L L
ATOM				24	127.232	59.442	44.174	1.00 50.30	L L
ATOM			HIS	25	125.154	60.295	44.359	1.00 48.84	Ŀ
ATOM			ALA		124.546	59.309	43.470	1.00 62.65	L
ATOM			ALA	25	123.334	58.678	44.149	1.00 50.68	L
ATOM	*		ALA	25	124.135	59.923	42.124	1.00 71.88	L
ATOM			ALA	25	124.135	61.098	42.053	1.00 69.35	L
ATOM			ALA	25	4	59.120	41.061	1.00 75.26	Ŀ
ATOM			SER	26	124.196	59.585	39.724	1.00 /5.26	L
ATOM			SER	26	123.833	58.421	39.724	1.00 53.25	L
ATOM			SER	26	123.832		38.981	1.00 34.32	L
ATOM			SER	26	122.779	57.511	39.755	1.00 54.52	L
ATOM	:		SER	26	122.466	60.247	39.733	1.00 70.72	Ŀ
ATOM	:		SER	26	122.329	61.422	40.163	1.00 70.72	ь Г
ATOM		•	GLN	27	121.452	59.490	•	1.00 /0.13	Tr Tr
ATOM		,a	GLN	27	120.103	60.030	40.253		L
ATOM			GLN	27	119.171	59.312	39.273 39.181	1.00 49.30 1.00 40.46	L
ATOM	1		GLN	27	119.385	57.827	39.899	1.00 47.76	, L
ATOM			GLN	27	118.295 117.623	57.064 57.601	40.785	1.00 42.99	L
ATOM	1			27		55.806	39.523	1.00 42.33	L
ATOM			GLN	27	118.110	59.937	41.690	1.00 57.30	L
ATOM			GLN		119.568		42.623	1.00 58.99	. L
ATOM		•	GLN	27	120.323	59.658			, L
ATOM			ASN	28	118.268	60.160	41.859		Ľ
ATOM			ASN	28	117.628	60.162	43.176	1.00 48.17	L.
ATOM			ASN	28	116.286	60.871	43.058	1.00 28.87	
MOTA		,	ASN	28	115.671	61.159	44.397	1.00 25.62	L
ATOM				28	116.346	61.607	45.321	1.00 43.90	L
ATOM				28	114.383	60.894	44.518	1.00 47.96	L
ATOM			ASN	28	117.422	58.833	43.917	1.00 53.06	L T.
ATOM			ASN	28	116.727	57.939	43.431	1.00 50.76	L
ATOM	•		ILE	29	118.011	58.727	45.112	1.00 49.78	L
ATOM			ILE	29	117.887	57.528	45.951	1.00 48.76	L
ATOM			ILE	29	119.278	56.900	46.275	1.00 38.91	L
ATOM	20	5 CG2	LILE	29	119.870	56.276	45.028	1.00 38.09	Ŀ
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MOTA	206	CG1	·ILE	29	120.235	57.965	46.801	1.00 35.93	L
MOTA	207	· CD1	ILE	. 29	121.444	57.381	47.498	1.00 24.13	L
ATOM	208	C	ILE	29	117.176	57.883	47.270	1.00 49.01	L
MOTA	209	0	ILE	29	117.043	57.056	48.183	1.00 28.15	L
ATOM .	210	N	TYR	30	116.720	59.127	47.358	1.00 51.14	L
MOTA	211	CA ·	TYR	30	116.018	59.610	48.536	1.00 40.55	L
MOTA	212	CB	TYR	30	114.708	58.834	48.708	1.00 51.35	L,
MOTA	213	CG	TYR	30	113.856	58.829	47.452	1.00 50.82	L
ATOM	214	CD1	TYR	30	112.914	59.832	47.218	1.00 57.07	L
MOTA	215	CE1	TYR	30	112.164	59.859	46.044	1.00 48.93	Ŀ
ATOM	216	CD2	TYR	30	114.023	57.846	46.477	1.00 54.94	L
MOTA	. 217	CE2	TYR	30	113.280	57.863	45.302	1.00 54.60	L
ATOM	218	CZ	TYR	30	112.354	58.872	45.089	1.00 54.60	L
ATOM	219	OH	TYR	30	111.641	58.906	43.914	1.00 46.05	L
MOTA	220	C	TYR	30	116.867	59.539	49.800	1.00 36.49	Ŀ
MOTA	221	0	TYR	30	117.747	60.377	50.007	1.00 36.08	$\mathbf{L}_{\mathbf{I}}$
ATOM	222	N	VAL	31	116.607	58.553	50.650	1.00 27.22	Ŀ
ATOM	223	CA	VAL	31	117.363	58.421	51.889	1.00 25.88	L
ATOM	224	CB	VAL	31	116.518	58.771	53.103	1.00 24.60	${f L}$
MOTA	225	CG1	VAL	31	115.741	60.036	52.827	1.00 39.18	L
MOTA	226	CG2	VAL	31	115.581	57.607	53.441	1.00 11.43	\mathbf{L}
MOTA	227	C	VAL	31	117.815	57.001	52.068	1.00 30.74	\mathbf{r}
MOTA	228	0	VAL	31	118.333	56.637	53.125	1.00 32.26	L
MOTA	229	N	TRP	32	117.612	56.202	51.028	1.00 34.27	\mathbf{L}
MOTA	230	CA	TRP	32	117.978	54.796	51.064	1.00 29.66	\mathbf{L}
ATOM	231	CB	TRP	32	117.016	53.999	50.173	1.00 37.57	L
ATOM	232	CG	TRP	32	115.569	54.306	50.497	1.00 45.16	L
MOTA	. 233	CD2	TRP	32	114.858	53.921	51.677	1.00 28.80	\mathbf{L}
MOTA	234	CE2	TRP	32	113.571	54.493	51.597	1.00 36.20	. L
MOTA	235	CE3	TRP	32	115.183	53.149	52.798	1.00 25.93	L
MOTA	236	CD1	TRP	. 32	114.706	55.074	49.765	1.00 47.52	L
MOTA	237	NE1	TRP	32	113.504	55.193	50.418	1.00 36.87	L
MOTA	238	CZ2	TRP	3.2	112.610	54.319	52.591	1.00 25.25	- L
MOTA	239	· CZ3	TRP	32	114.229	52.978	53.788	1.00 21.98	L .
ATOM	240	CH2	TRP	32	112.954	53.563	53.677	1.00 2.00	Ŀ
MOTA	241	C ,	TRP	32	119.419	54.578	50.645	1.00 17.38	, L
ATOM	242	0	TRP	32	119.697	54.267	49.491	1.00 20.83	. <u>.</u>
MOTA	243	N	LEU	33	120.332	54.750	. 51.599	1.00 19.97	\mathbf{L}
MOTA	244	CA	LEU	` 33	121.763	54.570	51.357	1.00 39.54	L _i
MOTA	245	CB ·	LEU	33	122.352	55.790	50.642	1.00 44.19	L
MOTA	246	CG	LEU	33	123.876	55.803	50.500	1.00 34.32	L
MOTA	247	CD1	LEU	33	124.252	56.190	49.078	1.00 27.47	Ŀ
MOTA	248	CD2	LEU	33	124.479	56.774	51.515	1.00 19.98	L
MOTA	249	C	LEU	33 .	122.481	54.371	52.685	1.00 39.15	· L
ATOM		, O	LEU	33	122.345	55.182	53.595	1.00 42.09	L -
MOTA	251	N	ASN	34	123.262	53.303	52.785	1.00 38.96	<u>г</u>
ATOM	252	CA	ASN	34	123.969	53.008	54.017	1.00 33.81	L
MOTA	253	CB	ASN	34	123.635	51.588	54.470	1.00 29.67	L
MOTA	254	CG	ASN	34	122.323	51.104	53.908	1.00 18.96	L -
MOTA	255		ASN	34	121.252	51.484	54.384	1.00 22.09	<u>Г</u>
MOTA	256	ND2	ASN	34	122.396	50.269	52.883	1.00 22.68	L
ATOM	257	C	ASN	34	125.465	53.162	53.889	1.00 27.35	L
MOTA	258	0	ASN	34	125.996	53.215	52.785	1.00 25.60	L

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ATOM	259	N	TRP	3	5		126.125	53.242	55.041	1.00	31.00	Ŀ
ATOM	260	CA	TRP	3	5		127.574	53.380	55.122	1.00	37.04	\mathbf{L}
ATOM	261	CB.	TRP	. 3	5		127.942	54.663	55.871	1.00	44.59	L
MOTA	262	CG	TRP	3	5		127.725	55.956	55.099	1.00	50.73	L
ATOM	263	CD2	TRP	. 3		r	128.624	56.560	54.155	1.00	39.25	L
ATOM	264	CE2	TRP	3			128.042	57.776	53.738	1.00	36.81	L
ATOM	265	CE3	TRP	3			129.868	56.194	53.621	1.00	29.95	L
ATOM	266	CD1	TRP	3			126.660	56.808	55.208	1.00	38.58	·L
ATOM	267	NE1	TRP	3			126.843	57.900	54.397	1.00	40.14	Ŀ
ATOM	268	CZ2	TRP	3			128.655	58.629	52.812	1.00	36.05	L
ATOM	269	CZ3	TRP	3			130.479	57.045	52.698	1.00	39.51	L
ATOM	270	CH2	TRP	3			129.871	58.247	52.307	1.00	31.94	L
ATOM	271	C	TRP	3			128.118	52.168	55.885	1.00	32.85	L
ATOM	271	0	TRP	3			127.499	51.715	56.849	1.00		L
	273	И	TYR	3			129.271	51.654	55.451	1.00	29.03	, L
MOTA	273 274	CA	TYR	3			129.894	50.488	56.080	1.00	24.01	L
MOTA	274	CB	TYR	3			129.760	49.256	55.178	1.00	24.57	L
MOTA	275 276	СБ	TYR		6		128.341	48.844	54.845	1.00		r P
MOTA		CD1	TYR		6		127.740	47.745	55.469	1.00		L
MOTA	277				6		126.439	47.350	55.138	1.00		L
MOTA	278	CE1	TYR		о б		127.606	49.536		1.00		L L
ATOM	279	CD2	TYR		6		126.314	49.153	53.550	1.00		L L
ATOM	280	CE2	TYR				125.736	48.064	54.174	1.00	33.13	L
ATOM	281	CZ	TYR		6	K	124.458	47.709	53.810	1.00		L
ATOM	282	OH	TYR		6		131.379	50.683	56.401	1.00		L
ATOM	283	C .	TYR		6			51.530	55.813	1.00	31.84	L
ATOM	284	0	TYR		6		132.060	49.880	57.337	1.00	38.75	L
ATOM	. 285	N	GLN		7	•	131.876	49.923	57.731	1.00		· L
ATOM	286	CA	GLN		7		133.278	50.342	59.199	1.00		L
ATOM	287	CB	GLN		7		133.406	50.342	59.704	1.00		· L
ATOM	288	CG	GLN		7		134.852	50.332	61.222	1.00		L
ATOM	289	CD	GLN		7,		134.989	49.222	61.753	1.00		L
ATOM	290	OE1	GLN		7.		134.904	51.439	61.733	1.00		L
ATOM	291	NE2	GLN		7		135.209	48.528	57.528	1.00		L
ATOM	292	C	GLN		7		133.884	47.526	57.975	1.00		L
ATOM	293	0	GLN		7		133.319	47.526	56.839	1.00	ps.	L
ATOM	294	N	GLN		8		135.022	47.195	56.596	1.00		Ŀ
ATOM	295	CA	GLN		8	:	135.695	46.738	55.155	1.00		L
ATOM	296°	CB ·	GLN		8		135.471 136.385	45.597	54.724	1.00	-	L
MOTA	297	CG	GLN		8			44.992	53.401	1.00		L
ATOM	298	CD	GLN		8		135.973	45.693	52.399	1.00		L
ATOM	299	OE1			8	."	135.856	43.683	53.390	1.00		L
ATOM	300	NE2			8		135.753		56.860	1.00		L
ATOM	301	C	GLN		8		137.192	47.285		1.00		L
ATOM	302	0	GLN		8		137.952	47.630	55.963			Ŀ
ATOM	303		LYS		9		137.610	46.969	58.086	1.00		r T
MOTA	304	CA	LYS		9	- 1	139.021	47.022	58.464	1.00		I.
ATOM	305	CB	LYS		9		139.204		59.925	1.00		Ŀ
MOTA	306	CG	LYS		9		139.493	47.764	60.884	1.00	31.56	.L
ATOM	307	CD	LYS		9		138.268	48.135	61.72.7			L.
ATOM	308	CE	LYS		9		138.633	48.266	63.205	1.00		L
MOTA	309	NZ	LYS		9		137.922	47.293	64.094	1.00		L L
ATOM	310	C	LYS		9		139.831	46.103	57.566	1.00		
MOTA	311	- O	LYS	3	9		139.272	45.238	56.886	1.00	49.56	·L

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ATOM	312	N	PRO ·	.40	141.161	46.283	57.533	1.00 54.59	L
ATOM	313	CD.	PRO	40	141.957	47.289	58.266	1.00 52.22	Ŀ
MOTA	314	CA	PRO	40	142.007	45.434	56.686	1.00 54.43	, 'L
ATOM	315	CB	PRO	40	143.431	45.874	57.037	1.00 40.87	L
ATOM	316	CG	PRO	40	143.274	47.280	57.530	1.00 36.77	L
MOTA	317	C	PRO	40	141.792	43.935	56.895	1.00 53.33	L
MOTA	318	0	PRO	40	141.962	43.429	58.003	1.00 48.18	L
ATOM	319	N	GLY	41 .	141,.403	43.244	55.825	1.00 56.47	L
ATOM	320	CA	GLY	41	141.178	41.807	55.889	1.00 46.36	Ŀ
MOTA	321	C	GLY	41	140.030	41.378	56.783	1.00 47.51	Ŀ
ATOM	322	0	GLY	41	139.890	40.195	57.103	1.00 42.82	L
ATOM	323	N	ASN	42	139.198	42.336	57.177	1.00 39.14	L.
ATOM	324	CA	ASN	42	138.061	42.049	58.044	1.00 33.16	Ŀ
ATOM	325	CB	ASN	42	138.031	43.041	59.210	1.00 25.23	Ŀ
ATOM	326	CG	ASN	42	137.400	42.453	60.451	1.00 34.65	L
ATOM	327	OD1	ASN	42	136.876	41.338	60.416	1.00 42.65	Ŀ
MOTA	328	ND2	ASN	42	137.444	43.194	61.558	1.00 15.22	L
MOTA	329	C	ASN	42	136.743	42.123	57.287	1.00 36.43	L
ATOM	330	0	ASN	42	136.726	42.413	56.092	1.00 31.10	L
MOTA	331	N	ILE	43	135.648	41.852	57.993	1.00 46.04	L
ATOM	332	CA	ILE	43	134.310	41.894	57.407	1.00 55.78	L
MOTA	333	CB	ILE	43	133.340	40.879	58.089	1.00 55.57	L
ATOM	334	CG2	ILE	43	134.038	39.554	58.323	1.00 47.83	L
MOTA	335	CG1	ILE	43	132.828	41.439	59.423	1.00 61.00	L
ATOM	336	CD1	ILE	43	131.656	40.662	60.017	1.00 68.36	Ŀ
MOTA	337	C	ILE	43	133.726	43.298	57.555	1.00 63.83	L
MOTA	338	0	ILE	43	134.037	44.010	58.513	1.00 72.13	Ŀ
MOTA	339	N	PRO	44	132.881	43.720	56.605	1.00 56.85	Li
MOTA	340	CD	PRO 4	44	132.444	42.988	55.402	1.00 59.76	T,
MOTA	341	CA	PRO	44	132.282	45.052	56.681	1.00 47.82	L
MOTA	342	CB	PRO	44	131.893	45.349	55.242	1.00 52.95	L
MOTA	343	CG.	PRO	44	131.590	43.997	54.665	1.00 66.17	· "L
MOTA	344	C	PRO	44	131.079	45.064	57.613	1.00 41.70	L
MOTA	345	0	PRO	44	130.160	44.258	57.460	1.00 35.22	L
ATOM	346	N	LYS	45	131.095	45.982	58.575	1.00 33.96	L
MOTA	347	CA	LYS	45	130.010	46.106	59.537	1.00 39.65	L
MOTA	348	CB	LYS	45	130.576	46.225	60.953	1.00 36.05	L
MOTA	349	CG	LYS	45	132.096	46.222	61.012	1.00 44.96	上
ATOM	350	CD	LYS	45	132.651	45.003	61.752	1.00 53.54	$oldsymbol{\Gamma}$
MOTA	351	CE	LYS	45	134.060	45.269	62.297	1.00 58.35	L
MOTA	352	NZ	LYS	45	134.818	44.011	62.586	1.00 46.04	Ŀ
ATOM	353	C	LYS	45	129.162	47.329	59.218	1.00 37.07	Lı
ATOM	354	0	LYS	.45	129.686	48.369	58.817	1.00 37.21	L
ATOM	355	N	LEU	46	127.850	47.205	59.385	1.00 22.26	L
ATOM	356	CA	LEU	46	126.969	48.326	59.107	1.00 28.40	T.
ATOM	357	CB	LEU	46	125.505	47.904	59.239	1.00 32.99	L
ATOM	358	CG '	LEU	46	124.429	48.756	58.541	1.00 40.56	L
ATOM .	359	CD1	LEU	46	123.264	48.947	59.508	1.00 53.21	L _
MOTA	360	CD2	LEU	46	124.987	50.114	58.096	1.00 41.53	. L
MOTA	361	C	LEU	46	127.268	49.459	60.079	1.00 27.28	L -
ATOM	362	0	LEU	46	127.353	49.247	61.286	1.00 40.74	Li -
MOTA	363	N	LEU	47	127.414	50.666	59.548	1.00 31.54	L
ATOM	364	CA	LEU	47	127.719	51.837	60.362	1.00 26.31	L

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•	MOTA	1 1	365	CB	LEU .	47	•	128.915	52.562	59.755	1.00	25.09	2 4	Ŀ
	MOTA		366	CG	LEU	47		130.100	52.926	60.636	1.00	16.21		Ŀ
	MOTA		367	CD1	LEU	47		130.727	51.676	61.198	1.00	17.63		Ŀ
	MOTA		368	CD2	LEU	47		131.094	53.701	59.805	1.00	2.00		L ·
	MOTA		369	C	LEU	47	,	126.535	52.807	60.449	1.00	34.89		Ŀ
	MOTA		370	0	LEU	47		126.190	53.282	61.535	1.00	26.31		L
	MOTA		371	N	ILE	48		125.934	53.100	59.293	1.00	44.65		L
	MOTA		372	CA	ILE	48		124.794	54.018	59.187	1.00	34.33		L
	MOTA		373	CB	ILE	48		125.251	55.439	58.788	1.00	24.64		L
	ATOM		374	CG2	ILE	48		124.145	56.146	58.008	1.00	29.43		L
	MOTA		375	CG1	ILE	48		125.591	56.253	60.033	1.00	28.98		· L
	MOTA	•	376 [.]	CD1	ILE	48		126.967	56.866°	59.993	1.00	25.03	•	L
	MOTA	٠	377	C	ILE	48		123.775	53.576	58.133	1.00	29.31		L
	MOTA		378	0	ILE	48		124.113	53.411	56.962	1.00	40.59		L
	MOTA		379	N	TYR	49		122.527	53.405	58.547	1.00	15.91		$\mathbf{T}^{\mathbf{r}}$
	MOTA		380	CA	TYR	49		121.485	53.018	57.613	1.00	21.27		L
	MOTA		381	CB	TYR	49		120.762	51.748	58.087	1.00	36.34	-	\mathbf{L}
	MOTA		382	CG	TYR	49		119.779	51.925	59.231	1.00	35.16		L
	ATOM		383	CD1	TYR	49		118.408	52.066	58.986	1.00	25.01		Ŀ
	ATOM		384	CE1	TYR	49		117.498	52.216	60.028	1.00	28.72		L
	ATOM		385	CD2	TYR	49		120.214	51.934	60.560	1.00	28.85		L
	ATOM		386	CE2	TYR	49		119.308	52.084	61.614	1.00	30.37		\mathbf{L}
	ATOM		387	$\mathbf{C}\mathbf{Z}$	TYR	49	,	117.953	52.228	61.340	1.00	42.99		L.
	MOTA		388	ОН	TYR	49	-	117.048	52.410	62.370	1.00	55.09	Ŧ	Ŀ
	ATOM		389	C	TYR	49		120.510	54.172	57.486	1.00	24.72		L
	ATOM	,	390	O	TYR	49		120.451	55.037	58.356	1.00	26.69		L
	MOTA	•	391	N	LYS	50		119.762	54.189	56.392	1.00	25.34	:	L
	ATOM		392	CA	LYS	50	**	118.786	55.241	56.132	1.00	19.61		L
	ATOM		393	CB	LYS	50		117.611	55.134	57.108	1.00	42.59	:	L
	ATOM	•	394	CG	LYS	50		116.426	54.345	56.566	1.00	36.91	**	L
	ATOM		395	CD	LYS	50		115.124	55.118	56.723	1.00	40.28		L
	ATOM		396	CE	LYS	50		114.289	54.568	57.865	1.00	33.03	1	$\mathbf{L}_{\mathbf{i}}$
	ATOM		397	NZ	LYS	50		112.829	54.799	57.659	1.00	38.05	r	\mathbf{L}
	ATOM		398	C	LYS	50		119.368	56.645	56.192	1.00	22.01		Ŀ
	MOTA	:	399	0	LYS	50	"	118.697	57.575	56.623	1.00	30.12		L
ź	ATOM	ŧ	400	N	ALA	51		120.622	56.790	55.779	1.00	32.92		L
	ATOM		401	CA	ALA	51		121.275	58.094	55.749	1.00	27.76		L
	ATOM		402	CB	ALA	51	•	120.346	59.117	55.100	1.00	14.79	*	L
	MOTA	•	403	C	ALA	51		121.787	58.647	57.073	1.00	25.18		L
	ATOM		404	0	ALA	51		122.949	59.026	57.173	1.00	28.58		L
	ATOM	r	405	\mathbf{N} .	SER	52		120.927	58.714	58.081	1.00	22.15		L
	ATOM	•	406	CA	SER	52		121.347	59.270	59.362	1.00	19.39		L
	ATOM	,	407	CB	SER	52		120.690	60.632	59.599	1.00	25.09		L
	MOTA		408	OG	SER	52		120.199	61.188	58.390	1.00	53.81		L
	MOTA		409	C .	SER	52		121.021	58.369	60.518	1.00	20.68		L
	ATOM		410	0	SER	52		121.232	58.729	61.674	1.00	23.62		Ŀ
	MOTA		411	N	ASN	53		120.497	57.194	60.209	1.00	25.87		L
	ATOM	r	412	CA	ASN	53		120.157	56.253	61.254	1.00	27.39	r	L
	MOTA		413	CB	ASN	53	z	118.992	55.387	60.811	1.00	27.54	:	L
	ATOM		414	CG	ASN	53		117.668	55.895	61.323	1.00	28.84	•	Ŀ
٠	ATOM		415	OD1	ASN	53		116.619	55.656	60.729	1.00	26.55		Ŀ
	ATOM		416	ND2	ASN	53		117.713	56.607	62.450	1.00	36.37		L
	ATOM		417	С	ASN	53		121.366	55.402	61.592	1.00	25.27		L
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ATOM	418	0	ASN	53	121.809	54.592	60.783	1.00	34.60	L
ATOM	419	N	LEU	54	121.899	55.607	62.795	1.00	34.99	L
ATOM	420	CA	LEU	54	123.064	54.880	63.294	1.00	47.12	L
ATOM	421	CB	LEU	54	123.649	55.607	64.510	1.00	37.02	. L
ATOM	422	CG	LEU	54	125.152	55.873	64.594	1.00	20.40	Ŀ
ATOM	423	CD1	LEU	54	125,508	57.117	63.830	1.00	25.30	L
MOTA	424	CD2	LEU	54	125.533	56.034	66.039	1.00	22.53	L
ATOM	425	C	LEU	54	122.660	53.468	63.705	.1.00	56.63	L
ATOM	426	0	LEU	54	121.529	53.250	64.145	1.00	68.94	Ŀ
ATOM	427	. N	HIS	55 ·	123.578	52.513	63.573	1.00	51.79	L
MOTA	428	CA	HIS	55	123.267	51.142	63.948	1.00	38.57	. L
ATOM	429	CB	HIS	55	124.091	50.139	63.137	1.00	36.54	L
ATOM	43.0	CG	HIS	55	123.551	48.742	63.186	1.00	27.93	L
ATOM	431	CD2	HIS	55	122.338	48.268	63.551	1.00	31.02	L
	432	ND1	HIS	55	124.303	47.639	62.841	1.00	36.74	L
ATOM		CE1	HIS	55	123.573	46.545	62.993	1.00	43.03	Ŀ
ATOM	433	NE2	HIS	55	122.376	46.902	63.423	1.00	37.77	L
MOTA	434		HIS	55	123.513	50.925	65.424	1.00	38.01	L
ATOM	435	C O	HIS	55	124.296	51.634	66.058	1.00	47.97	Ŀ
ATOM	436	_		56	122.832	49.930	65.966	1.00	33.15	L
ATOM	437	N	THR	56	122.951	49.600	67.371	1.00	41.46	L
ATOM	438	CA	THR	56	122.008	48.436	67.708	1.00	58.72	L
ATOM	439	CB	THR	56	121.601	47.787	66.495	1.00	57.81	L
ATOM	440	OG1		56 56	120.770	48.955	68.430	1.00	63.75	L
ATOM	441	CG2	THR	56	124.380	49.260	67.805	1.00	32.47	L
ATOM	442	C	THR		124.940	48.236	67.415	1.00	23.36	L
ATOM	443	0	THR	56 ·	124.967	50.136	68.612	1.00	28.03	L
ATOM	444	N	GLY	57	126.311	49.893	69.101	1.00		L L
ATOM	445	CA	GLY	57 57	127.388	50.703	68.403	1.00		L
ATOM	446	C	GLY	57 57	128.584	50.506	68.641	1.00		, Li
MOTA	447	0	GLY	57	126.971	51.616	67.537	1.00		L
ATOM	448	N	VAL	58	127.926	52.439	66.819		42.70	
ATOM	449	CA	VAL	58 50	127.448	52.680	65.372	1.00		. <u> </u>
ATOM	450	CB	LAV	58 50	128.383	53.648	64.654		20.54	L _i
ATOM	451	CG1		58 50	127.380	51.354	64.635	1.00		L
ATOM	452	CG2		58 58	128.129	53.768	67.546	1.00		L L
ATOM	453	C	VAL	58	127.178	54.509	67.780	1.00		L L
ATOM	454	0	VAL	58	127.178	54.059	67.951	1.00		L
ATOM	455	N	PRO	59	130.553	53.187	67.788	1.00		 . L
ATOM	456	CD	PRO	59	129.717	55.296	68.658	1.00		L
ATOM	457	CA	PRO	59	131.253	55.289	68.706	1.00		L
ATOM	458	CB	PRO	59 50	131.698	54.148	67.847	1.00	_	Ţ.
ATOM	459	CG	PRO	5 <i>9</i>	129.174	56.543	67.980	1.00	**	L.
ATOM	460	C	PRO	59 50	129.174	56.694	66.762	1.00		L
ATOM	461	0 ,	PRO	59		57.437	68.782	1.00		L L
MOTA	462	N	SER	60	128.605	58.680	68.274	1.00		L
MOTA	463	CA	SER	60	128.044		69.424	1.00		L
MOTA	464	CB	SER	60	127.466	59.513	70.648	1.00		L
MOTA	465	OG	SER	60	128.108	59.201			33.70	L
MOTA	466	C	SER	60	129.096	59.492	67.536	1.00		L
MOTA	467	0	SER	60	128.760	60.405	66.785	1.00		Ŀ
ATOM	468	N	ARG	61	130.369	59.175	67.758			L
MOTA	469	CA	ARG	61	131.440	59.887	67.068	1.00		
ATOM	470	· CB	ARG	61	132.801	59.241	67.361	1.00	45.69	נג

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ATOM	•	471	CG	ARG	61	133.316	58.277	66.278	1.00	69.44	Ĺ,
ATOM		472	CD ·	ARG	61	134.854	58.263	66.188	1.00	56.63	L
MOTA		473	NE	ARG	61	135.482	57.895	67.458	1.00	41.22	L
ATOM		474	$\mathbf{C}\mathbf{Z}^{'}$	ARG	61	135.733	56.646	67.834	1.00	36.39	L
ATOM		475	NH1	ARG	61	135.411	55.637	67.041	1.00	46.50	· L
ATOM		476	NH2	ARG	61	136.294	56.405	69.008	1.00	45.10	L
ATOM		477	C	ARG	61.	131.137	59.822	65.573	1.00	39.44	Ŀ
MOTA		478	0	ARG .	61	131.495	60.718	64.807	1.00	31.59	L
MOTA		479	N	PHE	62	130.468	58.744	65.176	1.00	29.20	L
MOTA		480	CA	PHE	62	130.083	58.534	63.795	1.00	21.62	L .
MOTA		481	CB	PHE	62	129.922	57.038	63.507	1.00	15.95	1
MOTA		482	CG	PHE	62	131.216	56.325	63.248	1.00	28.60	L,
MOTA		483	CD1	PHE	62	131.770	56.303	61.975		25.81	Ŀ
MOTA		484	CD2	PHE	62	131.884	55.661	64.277	1.00	34.71	. L i
MOTA		485	CE1	PHE	62	132.973	55.629	61.730	1.00	25.28	L
MOTA		486	CE2	PHE	62	133.086	54.987	64.039	1.00	17.13	Ŀ
MOTA		487	CZ	PHE	62	133.628	54.972	62.759	1.00	16.17	L
ATOM		488	C	PHE	62	128.749	59.223	63.574	1.00	27.58	Li ~
MOTA		489	0	PHE	62	127.812	59.041	64.347	1.00	26.02	L -
MOTA		490	N	SER	63	128.667	60.028	62.526	1.00	27.01	<u>r</u>
MOTA		491	CA	SER	63	127.432	60.724	62.194	1.00	29.21	L ~
MOTA		492	CB	SER	63	127.512	62.197	62.620	1.00	27.06	L -
MOTA		493	OG	SER	63 ,	127.604	63.059	61.501	1.00	46.67	Ŀ
MOTA		494	C	SER	.63	127.271	60.609	60.689	1.00	31.69	L:
MOTA		495	0	SER	63	128.247	60.359	59.983	1.00	35.00	L
MOTA		496	N	GLY	64	126.046	60.778	60.203	1.00	32.44	L
MOTA		497	CA	GLY	64	125.796	60.677	58.775	1.00	28.03	L
MOTA	*	498	\mathbf{C}	GLY	64	124.656	61.567	58.325		36.15	L T
MOTA		499	0	GLY	64	123.678	61.753	59.050	1.00	31.20	L
MOTA	Y.	500	N	SER	65	124.761	62.103	57.115		45.47	L
MOTA		501	CA	SER	65	123.723	62.993	56.612	1.00	43.02	L
MOTA		.502	CB	SER	65	124.029	64.412	57.075	1.00	39.26	L
MOTA		503	OG -	SER	65	125.378	64.487	57.510		49.79	L
MOTA	e.	504	C	SER	65	123.566	62.975	55.097		33.50	L L
ATOM	, ,	505	0	SER	65	124.401	62.428	54.373	1.00	35.77 17.16	L
ATOM		506	N	GLY	66	122.485	63.579	54.625	1.00	29.10	L
ATOM		507	CA	GLY	66	122,258	63.641 63.081	53.196 52.769	1.00	35.42	· L
ATOM		508	C	GLY	66	120.920	62.267	53.479		32.46	Ŀ
ATOM		509	0	GLY '	66.	120.321	63.527	51.608		24.62	L
ATOM	•	510	N	SER	67		63.062	51.061		28.74	L
ATOM		511	CA	SER	67	119.184	63.757	51.757		46.75	Ĺ
ATOM	*	512	CB	SER -	67	118.012	63.757	51.757		59.32	L
ATOM		513	OG	SER	67	116.780	63.343	49.567			L:
ATOM		514	C	SER	67	119.129	64.391	49.113		35.08	L
ATOM		515	0	SER	67	119.579		48.803	1.00		Ti Ti
ATOM		516	N	GLY	68	118.589	62.399 62.585	47.367		22.78	Ŀ
ATOM		517	CA	GLY	68	118.485			1.00		L
MOTA		518	C		· 68	119.712	62.129 60.935	46.604 46.341	1.00		Ŀ
MOTA		519	O 2T	GLY	68	119.885	63.086	46.255	1.00	36.67	L
MOTA	ı	520	N	THR	69	120.567		45.505	1.00	36.14	Ŀ
MOTA		521	CA	THR	69	121.784	62.805			43.08	Ŀ
ATOM		522	CB	THR	69	121.890	63.748	44.285			r L
ATOM		523	OGl	THR	69	120.775	63.516	43.414	Τ.00	47.12	Ц

			*	p ¹ = ±	: 1	1	P P ₁ = 1			, , ,		. 4
MOTA	524	CG2	THR	69		123.175	63.505	43.514	1	44.41		L
ATOM	525	C	THR	69		123.029	62.953	46.376	1.00	29.87	4 ,	L
ATOM	526	0	THR	69		123.915	62.101	46.350	1.00	38.58		Ŀ
ATOM	527	\cdot M	GLY	70 -		123.082	64.022	47.160	1.00	31.63		L
ATOM	528 ⁻	CA	GLY	70		124.234	64.256	48.016	1.00	42.61	" ,	L
ATOM	529	C	GLY	70		124.171	63.521	49.337	1.00	36.70		L
ATOM	530	0	GLY	70	٠	123.119	63.471	49.965	1.00	45.53	7	L
ATOM	531	\mathbf{N}	PHE	71		125.295	62.944	49.755	1.00	38.83		L ·
ATOM	532	CA	PHE	71		125.370	62.206	51.019	1.00	33.73		L
ATOM	533	CB	PHE	71		124.999	60.739	50.798	1.00	31.54		L
ATOM	534	CG	PHE	71		123.602	60.540	50.263	1.00	38.58		Ŀ
ATOM	535	CD1	PHE	71		122.561	60.199	51.120	1.00	21.48		L
MOTA	536	CD2	PHE	71		123.329	60.697	48.908	1.00	26.22		L
ATOM	537	CE1	PHE	71		121.278	60.021	50.641	1.00	26.37		L
ATOM	538	CE2	PHE	71		122.044	60.520	48.422	1.00	42.61		Ŀ
ATOM	539	CZ	PHE	71		121.016	60.183	49.286	1.00	24.00		L
ATOM	540	C	PHE	71		126.774	62.296	51.605	1.00	27.97		L
ATOM	541	0	PHE	71		127.760	62.212	50.877	1.00	31.31		L
ATOM	542	N	THR	72		126.866	62.457	52.921	1.00	26.78		L
ATOM	543	CA	THR	72		128.167	62.582	53.564	1.00	26.67		L,
ATOM	544	CB	THR	72		128.520	64.069	53.781	1.00	32.81		L
ATOM	545	OG1	THR	72		129.493	64.187	54.826	1.00	56.77		L
ATOM	546	CG2	THR	72		127.288	64.856	54.164	1.00	32.03		L
ATOM	547	C	THR	72	Ŷ	128.291	61.866	54.903	1.00	27.04	:	L
ATOM	548	0	THR	. 72	·	127.308	61.722	55.635	1.00	23.90		L
ATOM	549	N	LEU	73		129.511	61.417	55.207	1.00	31.55		Lì
ATOM	550	CA	LEU	73		129.816	60.722	56.459	1.00	24.92		L
ATOM	551	CB	LEU	73		130.387	59.333	56.194	1.00	32.89	,	L
ATOM	552	CG	LEU	73		130.625	58.551	57.490	1.00	34.57		L
ATOM	553	CD1	LEU	73,		129.287	58.045	58.021	1.00	14.98	4	L
ATOM	554	CD2	LEU	. 73	*	131.586	57.404	57.246	1.00	10.86		L
MOTA	555	C	LEU	73	•	130.826	61.512	57.274	1.00	25.60		${f L}$
ATOM	556	0	LEU	73		131.823	62.004	56.755	1.00	39.03		L
ATOM	557	N	THR	74	٠	130.581	61.593	58.567	1.00	21.07		L
ATOM	558	CA	THR	74		131.443	62.362	59.436	1.00	25.98		L
ATOM	559	CB	THR	74		130.686	63.625	. 59.933	1.00	34.99		L
ATOM	560	OG1	THR	74		130.181	64.351	58.808	1.00	35.85		L
ATOM	561	CG2	THR	74	, .	131.588	64.524	60.747	1.00	27.11	•	L
ATOM	562	C	THR	74	·	131.886	61.542	60.640	1.00	29.95		L
ATOM	563	0	THR	74.		131.065	60.931	61.322	1.00	36.77	:	L
ATOM	564	. N	·ILE	75		133.186	61.522	60.896	1.00	24.95	,	. L.
ATOM	565	CA	ILE	: 75	<u>.</u>	133.706	60.813	62.052	1.00	23.49		L
ATOM	566	CB	ILE	75	•	134.723	59.737	61.659	1.00	21.59	•	L
ATOM	567	CG2		75		135.597	59.401	62.847	1.00	7.06	ż	L
ATOM	568	CG1		75	•	133.988	58.479	61.198	1.00	33.47	1	· L
ATOM	569	CD1		75	•	133.840	58.343	59.687	1.00	25.94		\mathbf{L}_{1}
ATOM	570	C	ILE	75		134.399	61.855	62.914	1.00	34.16		L
ATOM	571	0	ILE	75		135.440	62.381	62.537	1.00	28.63		\mathbf{L}
ATOM	572	N	SER	76		133.803	62.167	64.05.9	1.00	42.00		L
MOTA	573	CA	SER	76		134.366	63.155	64.971	1.00	51.91		L
ATOM	574	CB	SER	76		133.251	63.762	65.829	1.00	67.85		L
ATOM	575	OG	SER	76		131.981	63.244	65.449	1.00	75.08		L
ATOM	576	C	SER	76		135.424	62.507	65.865	1.00	55.79	:	L
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•	ATOM	577 [*]	Ö A	SER	76	135.372	61.304	66.131	1.00 54.31	\mathbf{L}_{\cdot}
	ATOM	578	N	SER	77	136.384	63.307	66.319	1.00 51.60	L
	MOTA	579	CA	SER	77	137.459	62.818	67.177	1.00 51.14	L
	MOTA	580	CB	SER	77	136.993	62.788	68.633	1.00 51.40	L
	ATOM	581	O.G	SER	77	136.336	63.998	68.967	1.00 52.89	L
	ATOM	582	C	SER	77	137.938	61.433	66.755	1.00 49.10	L
	MOTA	583	0	SER	77	137.515	60.422	67.311	1.00 47.48	L
	MOTA	584	N	LEU	78 .	138.832	61.406	65.771	1.00 46.54	L
	MOTA	585	CA	LEU	78	139.389	60.168	65.241	1.00 32.83	L
	MOTA	586	CB	LEU	78	140.333	60.495	64.084	1.00 27.78	L
	MOTA	587	CG	LEU	78	140.423	59.481	62.950	1.00 35.44	L
	MOTA	588	CD1	LEU	78	139.472	59.898	61.855	1.00 40.91	L
	MOTA	589	CD2	LEU.	78	141.852	59.397	62.421	1.00 25.57	L
	ATOM	590	C	LEU	78	140.134	59.314	66.268	1.00 28.27	Ŀ
	MOTA	591	0	LEU	78	140.668	59.809	67.264	1.00 19.55	L
	ATOM	592	N	GLN	79	140.163	58.016	65.999	1.00 30.85	L
	MOTA	593	CA	GLN	79	140.847	57.064	66.859	1.00 34.63	L
	MOTA	594	CB	GLN	79	139.855	56.338	67.763	1.00 47.40	Ŀ
	MOTA	595	CG	GLN	79	139.162	57.238	68.764	1.00 66.32	L
	MOTA	596	CD	GLN	79	140.118	57.793	69.791	1.00 51.70	L
	ATOM	597	OE1	GLN	79	141.184	57.229	70.022	1.00 38.18	Ŀ
	MOTA	598	NE2	GLN	79	139.740	58.901	70.419	1.00 50.52	L
	ATOM	599	C	GLN	79	, 141.534	56.054	65.965	1.00 36.58	L
	MOTA	600	0	GLN	79	141.056	55.755	64.869	1.00 30.40	L
	MOTA	601	N	PRO	80	142.663	55.504	66.430	1.00 40.78	, L
	MOTA	602	CD	PRO	80 -	143.270	55.791	67.740	1.00 37.68	L
	ATOM	603	CA	PRO	80	143.430	54.513	65.665	1.00 41.10	Ъ
	MOTA	604	CB	PRO	80 -	144.460	53.991	66.672	1.00 43.39	L
	MOTA	605	CG	PRO	80	144.056	54.557	68.021	1.00 37.64	. L
:	ATOM	606	C.	PRO	80	142.532	53.398	65.149	1.00 46.35	· L
	ATOM .	607	O .	PRO	80	142.569	53.048	63.969	1.00 41.86	Ŀ
ž	MOTA	608	N	GLU -	81	141.72	52.859	66.056	1.00 57.27	L
	MOTA	609	CA	GLU	81	140.793	51.773	65.761	1.00 58.29	L -
	MOTA	610	CB	GLU	81	139.870	51.548	66.967	1.00 54.76	L
	ATOM	611	CG	GLU	81	138.677		67.042	1.00 71.46	L _i
	ATOM	612	CD	GLU	81	138.507	•	68.419	1.00 74.52	. L
	ATOM	613	OE1	GLU	81	137.390	_	68.983	1.00 60.52	. <u>L</u>
	MOTA	614	OE2	GLU	81	139.489		68.934	1.00 65.39	T ₁
	MOTA	615	C	GLU	81	139.956	-	64.503	1.00 62.35	L
·	MOTA	616	0	GLU	81			63.794	1.00 64.51	L
	MOTA	617	N	ASP	82	139.629		64.230	1.00 63.68	. L
	MOTA	618	CA	ASP	82	138.823		63.069	1.00 50.22	
	MOTA	619	CB	ASP	82 -	138.299		63.212	1.00 50.14	L
	ATOM	620	CG	ASP	82	137.729	55.285	64.581	1.00 50.17	. <u>L</u>
**	MOTA	621	OD1	ASP	82 .	137.10		65.143	1.00 56.15	Ŀ
	MOTA	622	OD2	ASP	82	137.90		65.095	1.00 62.15	. L
	MOTA	623	C	ASP	82	139.583		61.761	1.00 47.40	L
	MOTA	624	0	ASP	82 ·	139.080		60.706	1.00 44.58	L
	ATOM	625	N	ILE	83	140.80		61.830	1.00 43.70	L
	MOTA	626	CA	ILE	83	141.586		60.621	1.00 38.44	L
	MOTA	627	CB	ILE	83	142.99		60.932	1.00 41.83	Ŀ
	ATOM	628	CG2	ILE	83	143.42		59.846	1.00 41.86	L
	ATOM	629	CG1	ILE	83	143.982	2 53.356	61.025	1.00 52.87	L
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MOTA	630	CD1	ILE	83	145.232	53.032	61.826	1.00 47.10	\mathbf{L}_{i}
MOTA	631	C	ILE	83	140.827	51.706	59.794	1.00 32.55	ĻL
MOTA	632	0	ILE	83	140.588	50.594	60.263	1.00 26.83	· L
MOTA	633	N	ALA	84	140.441	52.085	58.575	1.00 26.12	L
MOTA	634	CA	ALA	84	139.692	51.200	57.693	1.00 15.10	· L
ATOM	635	СВ	ALA	84	138.453	50.702	58.406	1.00 21.07	Ŀ
MOTA	636	C	ALA	84	139.290	51.913	56.414	1.00 12.91	Ŀ
MOTA	637	0	ALA	84	139.668	53.060	56.195	1.00 24.44	L
MOTA	638	N	THR	85	138.519	51.224	55.578	1.00 19.66	L
MOTA	639	CA	THR	85	138.025	51.774	54.320	1.00 17.95	Ŀ
MOTA	640	CB	THR	85	138.413	50.898	53.131	1.00 21.81	L
MOTA	641	OG1	THR	85	137.552	51.197	52.024	1.00 45.12	L
ATOM	642	CG2	THR	85	138.277	49.435	53.490	1.00 27.37	Ŀ
MOTA	643	C	THR	85	136.505	51.809	54.410	1.00 27.74	L
MOTA	644	0	THR	85	135.876	50.804	54.732	1.00 32.43	Ŀ
ATOM	645	N	TYR	86	135.914	52.960	54.116	1.00 37.25	Ŀ
MOTA	646	CA	TYR	86	134.469	53.109	54.213	1.00 33.34	L
MOTA	647	CB	TYR	86	134.153	54.363	55.028	1.00 25.32	L
ATOM	648	CG	TYR	86	134.852	54.381	56.372	1.00 28.51	L
MOTA	649	CD1	TYR	86	134.151	54.118	57.547	1.00 44.83	· L
ATOM	650	CE1	TYR	86	134.801	54.071	58.789	1.00 21.36	L
MOTA	651	CD2	TYR	86	136.226	54.607	56.467	1.00 14.36	L
MOTA	652	CE2	TYR	86	136.884	54.561	57.705	1.00 22.98	L
ATOM	653	. CZ	TYR	86	136.158	54.289	58.857	1.00 22.24	
ATOM	654	OH	TYR	86	136.786	54.210	60.072	1.00 25.93	L
MOTA	655	C	TYR	86	133.766	53.159	52.868	1.00 44.00	Lı
MOTA	656	0	TYR	86	134.164	53.908	51.975	1.00 50.72	L
MOTA	657	N	TYR	87	132.712	52.353	52.748	1.00 51.03	L
ATOM	658	CA .	TYR	87	131.910	52.248	51.526	1.00 48.37	, L
ATOM	659	CB	TYR	87	131.795	50.780	51.108	1.00 25.20	. L
ATOM	660	CG.	TYR	87	133.108	50.126	50.753	1.00 41.42	L
ATOM	661	CD1	TYR	87	133.551	50.080	49.427	1.00 38.02	Ŀ
ATOM	662	CE1	TYR	87	134.769	49.484	49.096	1.00 42.21	Ŀ
MOTA	663	CD2	TYR	87	133.918	49.555	51.742	1.00 33.37	Ŀ
MOTA	664	CE2	TYR	87	135.137	48.957	51.418	1.00 33.81	Ŀ
MOTA	665	CZ	TYR	87	135.555	48.929	50.096	1.00 23.95	L
MOTA	666	OH	TYR	87	136.771	48.380	49.779	1.00 34.33	L
ATOM	667	C	TYR	87	130.493	52.813	51.687	1.00 52.12	L _
MOTA	668	0	TYR	87	129.948	52.838	52.786	1.00 65.19	. <u>r</u>
ATOM	669	N	CYS	88	129.895	53.250	50.582	1.00 47.34	L
ATOM	670	CA	CYS	88	128.538	53.789	50.598	1.00 32.49	
ATOM	671	C.	CYS	88	127.715	52.920	49.661	1.00 32.31	Li -
ATOM	672 -	0	CYS	88	128.140	52.641	48.547	1.00 39.98	
MOTA	673	CB	CYS	88	128.530	55.233	50.093	1.00.33.98	· L
MOTA	674	SG	CYS	88	128.799	55.411	48.289	1.00 51.95	L L
ATOM	675	N	GLN	89	126.549	52.476	50.109	1.00 22.59	L
MOTA	676	CA	GLN	89	125.709	51.648	49.260	1.00 21.84	L
MOTA	677	CB	GLN	89	125.810	50.179	49.700	1.00 31.57	L
ATOM	678	CG	GLN	89	124.788	49.740	50.735	1.00 42.44	L
MOTA	679	CD.	GLN	89	123.613	48.982	50.132	1.00 34.76	L L
ATOM	680	OE1	GLN	89 .	122.664	48.637	50.834	1.00 26.74	L
ATOM	681	NE2	GLN	89	123.671	48.723	48.831	1.00 46.97	L
MOTA	682	C	GLN	89	124.262	52.131	49.287	1.00 25.45	L

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	ATOM	683	0 .	GLN	89.	· ·	123.783	52.603	50.313	1.00	20.31		L,
	ATOM	684	\mathbf{N}	GLN	90 .	1.	123.574	52.035	48.153	1.00	19.13	*	L
	ATOM	685	CA	GLN	90		122.183	52.457	48.096	1.00	19.46	,	L,
	ATOM	686	CB	GLN	90		121.882	53.162	46.769	1.00	22.24		L
	ATOM	687	CG	GLN	90		122.072	52.299	45.523	1.00	38.10	• "	L
	ATOM	688	CD	GLN	90		120.775	51.666	45.009	1.00	30.31		Ŀ
	ATOM	689	OE1	GLN	90		119.701	51.853	45.586	1.00	32.81		L,
	ATOM	690	NE2	GLN	90	**	120.878	50.908	43.921	1.00	28.00		L
	ATOM	691	C	GLN	90		121.257	51.250	48.267	1.00	30.72	•	L
	ATOM	692	0	GLN	90		121.556	50.143	47.801	1.00	25.46		L
	ATOM	693	N	GLY	91		120.137	51.473	48.951	1.00	34.63		L
	ATOM	694	CA	GLY	91		119.166	50.416	49.179	1.00	33.97	•	L
	ATOM	695	C	GLY	91		117.820	50.781	48.580	1.00	38.48		L
	ATOM	696	0	GLY	91		116.762	50.335	49.035	1.00	28.43		L
	ATOM	697	N	GLN	92		117.869	51.603	47.540	1.00	28.95		L
	ATOM	698	CA ·	GLN	92		116.668	52.043	46.868	1.00	29.94	**	L
	ATOM	699	CB	GLN	92		116.841	53.489	46.418	1.00	30.37		L
	ATOM	700	CG	GLN	92		115.571	54.307	46.498	1.00	39.02		Ŀ
	MOTA	701	CD	GLN	92		115.079	54.736	45.130	1.00	41.59		上
	ATOM	702	OE1	GLN	92		114.039	54.274	44.663	1.00	31.97		L
	ATOM	702	NE2	GLN	92	ı	115.829	55.621	44.479		59.08		L
	ATOM	703	C	GLN	92		116.352	51.144	45.680		41.66		L
	ATOM	70 4 705	0	GLN	92		115.495	50.267	45.782		33.85		L
	ATOM	705 706	N	THR	93	4	117.046	51.373	44.564	1.00	60.13		L
	ATOM	703	CA	THR	93		116.866	50.596	43.327	1.00	66.93		L
	ATOM	708	CB.	THR	93		117.639	51.242	42.149	1.00	78.05		L
	ATOM	709	OG1	THR	. 93		117.362	52.647	42.104	1.00	79.52		L
		710	CG2	THR	93		117.233	50.610	40.829	1.00	75.70		Ŀ
	ATOM ATOM	711	C	THR	93	**	117.391	49.180	43.539	1.00	59.06		L
	ATOM	712	0 .	THR	93		118.425	49.009	44.183		58.37		L
	ATOM	713	N	TYR	94		116.703	48.173	42.993		50.92		L
	ATOM	714	CA	TYR	94		117.127	46.791	43.209	1.00	52.81		L
	ATOM	715	CB	TYR	. 94		116.119	45.793	42.646		55.69		L
	ATOM	716	CG	TYR	94	٠	115.809	44.706	43.658	1.00	64.81		Ĺ
	ATOM	717	CD1	TYR	94		116.742	44.361	44.643	1.00	66.44		L
	ATOM	718	CE1	TYR	94	*	116.451	43.413	45.622	1.00	61.74		L
	ATOM	719	CD2	TYR	94		114.573	44.066	43.676	1.00	65.08		L
	ATOM	720	CE2	TYR	94		114.269	43.112	44.654	1.00	75.90		L
	ATOM	721	CZ	TYR	94	7	115.214	42.796	45.623	1.00	73.24		L
r	ATOM	722	OH	TYR	94		114.918	41.877	46.603	1.00	7100		L
	ATOM	723	C	TYR	94	**	118.530	46.372	42.797	1.00	58.78	ı	L
	ATOM	724	0	TYR	94		119.146	45.561	43.487	1.00	72.46		L
,	ATOM	725	N	PRO	95	,	119.045	46.851	41.650	1.00	50.22		L
	ATOM	726	CD	PRO	95		118.550	47.719	40.573	1.00	29.17		Ŀ
	MOTA	727	CA	PRO	95		120.412	46.375	41.404	1.00	45.68	,	L
	ATOM	728	CB	PRO	. 95		120.673	46.762	39.946	1.00	19.42	•	L
	ATOM	729	CG	PRO	. 95		119.780	47.938	39.712	1.00	25.27		L
	ATOM	730	C	PRO	95		121.286	47.156	42.398		43.53	,	Ŀ
	ATOM	· 731	0	PRO	95		121.936	48.131	42.027		52.07		L
	ATOM	732	· M	TYR	96		121.253	46.734	43.667				L
	ATOM	733	CA	TYR	96	,	122.000	47.378	44.748	1.00	29.95		Ŀ
	MOTA	734	CB	TYR	96		122.099	46.463	45.971	1.00	35.33		L
	MOTA	735	CG	TYR	96		120.833	46.317	46.792	1.00	28.60		L
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MOTA	736	CD1	TYR	96	120.678	45.244	47.663	1.00 33.58	\mathbf{L}
ATOM	737	CE1	TYR	96	119.523	45.087	48.430	1.00 23.02	L
ATOM	738	CD2	TYR	96	119.792	47.244	46.701	1.00 29.21	L
ATOM	739	CE2	TYR	96	118.625	47.096	47.466	1.00 29.26	Ŀ
ATOM	740	CZ	TYR	96	118.506	46.011	48.329	1.00 29.92	L
ATOM	741	OH	TYR	96	117.383	45.853	49.102	1.00 25.77	Ŀ
ATOM	742	C	TYR	96	123.392	47.712	44.281	1.00 29.68	Ŀ
ATOM	743	0	TYR	96	123.980	46.954	43.511	1.00 37.11	L
ATOM	744	\mathbf{N}	THR	.97	123.926	48.830	44.770	1.00 36.89	L
ATOM	745	CA	THR	97	125.259	49.280	44.372	1.00 40.63	L
ATOM	746	CB	THR	97	125.153	50.181	43.141	1.00 46.47	L
ATOM	747	OG1	THR	97	123.945	50.951	43.228	1.00 49.45	· L
ATOM	748	CG2	THR	97	125.123	49.342	41.874	1.00 48.22	${f L}$
ATOM	749	C	THR	97	126.017	50.049	45.458	1.00 34.47	L
ATOM	750	O ~	THR	97	125.473	50.975	46.062	1.00 27.32	L
ATOM	751	N	PHE	98	127.268	49:662	45.700	1.00 24.58	Ŀ
ATOM	752	CA	PHE	98	128.097	50.338	46.689	1.00 19.63	L
ATOM	753	CB	PHE	98	129.009	49.369	47.458	1.00 21.69	Ŀ
ATOM	754	CG	PHE	98	128.386	48.051	47.780	1.00 22.09	L
ATOM	755	CD1	PHE	98	128.078	47.719	49.098	1.00 28.14	L
ATOM	756	CD2	PHE	98	128.145	47.117	46.780	1.00 29.87	L
MOTA	757	CE1	PHE	98	127.543	46.481	49.409	1.00 20.31	L
MOTA	758	CE2	PHE	98	127.610	45.877	47.080	1.00 20.97	L
MOTA	759	CZ	PHE	98	127.308	45.556	48.397	1.00 35.93	· L
ATOM	760	C	PHE	98	128.994	51.317	45.947	1.00 27.49	L
MOTA	761	0	PHE	98	128.868	51.493	44.738	1.00 15.09	L
MOTA	762	N	GLY	99	129.912	51.931	46.689	1.00 32.03	Ŀ
ATOM	763	CA	GLY	99	130.839	52.878	46.106	1.00 37.27	L
ATOM	764	C	GLY	99	132.207	52.250	45.927	1.00 44.52	L
ATOM	765	O ,	GLY	99	132.319	51.038	45.717	1.00 42.71	· L i
ATOM	766	\mathbf{N}	GLY	100	133.246	53.077	46.008	1.00 42.44	L
MOTA	767	CA	GLY	100	134.600	52.584	45.848	1.00 51.35	L
ATOM	768	C	GLY	, 100	135.344	52.448	47.164	1.00 53.12	L
MOTA	.769 ·	0	GLY	100	136.390	51.791	47.241	1.00 49.35	_
MOTA	770	N	GLY	101	134.799	53.067	48.204	1.00 43.66	L
MOTA	771	CA	GLY	101	135.430	53.013	49.504	1.00 26.42	· L
MOTA	772	C	GLY	101	136.368	54.181	49.696	1.00 21.78	L
MOTA	773	0	GLY	101	136.710	54.886	48.747	1.00 23.28	L.
MOTA	774	\mathbf{N}	THR	102	136.787	54.392	50.933	1.00 17.65	Ŀ
ATOM	775	CA	THR	102	137.682	55.489	51.221	1.00 39.10	L
MOTA	776	CB .	THR	102	136.869	56.745	51.644		L L
ATOM	777	OG1	THR	102	137.738	57.731		1.00 42.53	L
MOTA	778	CG2	THR	102	135.780	56.357	52.630	1.00 55.18	L L
ATOM	779	C ·	THR	102	138.659	55.072	52.311	1.00 37.54	<u>L</u> .
ATOM	780	0	THR	102	138.295	54.948	53.478	1.00 44.36	, L
ATOM	781	\mathbf{N}	LYS	103	139.903	54.830	51.911	1.00 34.42	L
ATOM	782	CA	LYS	103	140.943	54.427	52.850	1.00 33.42	L
MOTA	783	CB	LYS	103	142.245	54.118	52.095	1.00 27.82	L
ATOM	784	CG	LYS	103	.143.518	54.210	52.937	1.00 32.59	L
ATOM	785	CD	LYS	103	144.038	55.649	53.036	1.00 39.07	L
MOTA	786	CE	LYS	103	145.366		53.790	1.00 45.98	L
ATOM	787	NZ	LYS	103	146.255	56.817	53.258	1.00 37.43	L
MOTA	788	C .	LYS	103	141.185	55.531	53.868	1.00 23.38	L

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MOTA	789	- O	LYS	103		140.842	56.687	53:637	1.00	30.72	· L
ATOM	790	N	LEU	104		141.770	55.171	55.002	1.00	32.38	L
ATOM	791	CA	LEU	104		142.077	56.159	56.021	1.00	38.59	Ŀ
ATOM	792	CB	LEU	104		140.904	56.368	56.966	1.00	25.66	Ĺ
ATOM	793	CG	LEU	104		141.378	57.265	58.113	1.00	32.02	. L
ATOM	794.	CD1	LEU	104		140.804	58.658	57.944	1.00	23.79	L
ATOM	795	CD2	LEU	.104		140.996	56.648	59.452	1.00	29.54	L
ATOM	796	C	LEU	104		143.300	55.784	56.841	1.00	45.89	L
ATOM	797	0	LEU	104		143.525	54.612	57.154	1.00	45.41	L
ATOM	798	N	GLU	105		144.080	56.799	57.197	1.00	40.34	\mathbf{L}
ATOM	799	CA	GLU	105		145.280	56.597	57.979	1.00	35.75	· L
ATOM	800	CB	GLU	105		146.510	56.674	57.064	1.00	52.11	${f L}$
ATOM	801	CG	GLU	105		147.798	57.154	57.728	1.00	69.87	${f L}$
ATOM	802	CD	GLU	105		148.876	57.513	56.712	1.00	84.87	L
ATOM	803	OE1	GLU	105		150.027	57.054	56.875	1.00	87.68	L
ATOM	804	OE2	GLU	105		148.578	58.251	55.748	1.00	91.43	L
ATOM	805	C	GLU	105		145.365	57.644	59.076	1.00	23.69	L
MOTA	806	0	GLU	105		145.640	58.804	58.808	1.00	36.93	L
7	807	N .	ILE	106		145.088	57.241	60.311	1.00	29.41	Ĺ
MOTA			ILE	106		145.199	58.168	61.425	1.00	38.27	Ŀ
ATOM	808	CA	ILE	106		144.723	57.513	62.769	1.00	40.94	L
ATOM	809	CB	ILE	106		145.030	56.026	62.766	1.00	31.48	L
ATOM	810	CG2		106		145.387	58.193	63.971	1.00	37.37	L
ATOM	811	CG1	ILE		-	144.571	59.336	64.579	1.00	27.37	上 上
ATOM	812	CD1	ILE	106		144.371	58.441	61.434	1.00	40.57	L
ATOM	813	C	ILE	106		147.497	57.506	61.438	1.00	41.72	L
MOTA	814	O	ILE	106	4	147.497	59.716	61.399	1.00	48.16	L L
MOTA	815	N	LYS	107	•	148.500	60.100	61.364	1.00	42.60	Ŀ
ATOM	816	CA	LYS	107	,	148.500	61.486	60.736	1.00	20.26	Ŀ
ATOM	817	CB	LYS	107			62.069	60.819	1.00	43.13	L
ATOM	818	CG ,	LYS	107		150.043	63.572	60.590	1.00	34.99	Ŀ
ATOM	819	CD	LYS	107		150.034	63.895	59.108	1.00	38.89	L
ATOM	820	CE	LYS	107		149.967			1.00	13.28	L L
ATOM	821	NZ	LYS	107		148.581	63.791	58.588		51.65	Ŀ
ATOM	822	C	LYS	.107		149.186	60.089	62.729	1.00	65.04	L
ATOM	823	0	LYS	107		148.643	60.592	63.713	1.00	52.66	Ŀ
ATOM	824	N	ARG	108		150.388	59.519	62.781	1.00	39.90	L
ATOM	825	CA	ARG	108		151.147	59.450	64.028	1.00	33.40	L
ATOM	826	CB	ARG	108		151.199	58.007	64.553			L
MOTA	827	CG	ARG	108		152.127	57.083	63.771	1.00		L L
MOTA	828	CD	ARG	108		152.649	55.957	64.635	1.00		
ATOM	829	NE	ARG	108		153.934	56.297	65.246	1.00	*	Ŀ
ATOM	830	CZ	ARG	108		154.303	55.928	66.471		34.06	L
ATOM	831	NHl		108		153.489	55.205	67.224		57.79	L
MOTA	832	NH2	ARG	108		155.484	56.280	66.947		31.28	L
ATOM	833	C	ARG	108		152.566	59.974	63.858	1.00		L
ATOM	834	0	ARG	108		153.071	60.102	62.733	ı	36.52	L
ATOM	835	N	ALA	109		153.193	60.271	64.996		49.39	L
MOTA	836	CA	ALA	109		154.557	60.774	65.040		56.62	Ŀ
MOTA	837	CB	ALA	109		155.042	60.822	66.479	1.00	33.22	Ĺ
ATOM	838	C	ALA	109		155.479	59.894	64.209	1.00	68.35	L
MOTA	839	0	ALA	109		155.350	58.667		1.00	79.99	L _
ATOM	840	N	ASP	110		156.403	60.524	63.492	1.00	75.21	· L
ATOM	841	CA	ASP	110		157.350	59.784	62.673	1.00	65.78	L

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TOM	894	CA PHE		168.671	37.145	58.423	1.00 22.76	L .	
TOM	893	N PHE	118	168.626	38.560	58.091	1.00 28.82	Ŀ	
TOM.		O ILE	117	169.467	39.212	60.076	1.00 40.81	· L	
rom	891	C ILE	117	169.039	39.484	58.952	1.00 32.15	L	
COM	890	CD1 ILE	. 117	171.461	41.525	55.63.2	1.00 18.50	L	
MOT	888 889	CG2 ILE	117 117	170.529	40.742	56.537	1.00 26.40	L	
MOT	887	CG2 TLE	117 117	170.299 171.426	41.040	58.848	1.00 28.48	Ŀ	
MOT	886	CA ILE		168.935	40.929	58.487 57.902	1.00 35.02	Ti Li	
MO	885	N ILE	117	168.547	41.726	59.641	1.00 40.79 1.00 35.02	L L	
MO	884	O SER	116	166.413	41.891	58.976	1.00 53.07	L	1
MOT	883	C SER	116	167.292	42.130	59.799	1.00 44.61	L	•
MO	882.	OG SER	116	165.653	42.932	63.068	1.00 58.23	, L	
'OM	881	CB SER	116	165.975	42.188	61.913	1.00 55.78	Li	,
MOJ	880		116	166.988	42.939	61.053	1.00 51.12	L	
COM	879	N SER	116	166.458	44.237	60.659	1.00 44.76	L	
MOT	877 878	C VAL O VAL	115 115	166.544 167.064	45.327	62.541	1.00 36.49	. L	
MOZ	876	CG2 VAL	115	166.470	48.555 45.324	59.338 61.424	1.00 30.46 1.00 38.71	L L	
MO	875	CG1 VAL	115	167.217	46.269	58.670	1.00 26.72	L T.	ı
MOT	874	CB VAL	115	166.973	47.210	59.839	1.00 46.96	L	
MOT	873	CA VAL	115	165.939	46.594	60.815	1.00 42.49	L	•
MOT	872	N VAL	115	165.488	47.596	61.7,69	1.00 36.33	L '.	
MOT	871	O THR	114	163.527	46.585	62.247	1.00 35.53	L	
'OM	870	C THR	114	164.322	47.515	62.406	1.00 42.88	, L	
'OM	869	CG2 THR	114	162.926	49.305	65.518	1.00 31.63	. L	•
MO	868	OG1 THR	114	162.504	47.153	64.511	1.00 38.54	·L	t
MO	867	CB THR	114	163.505	48.159	64.706	1.00 34.54	L	•
OM	866	CA THR	114	164.009	48.675	63.341	1.00 39.49	${f L}$	r :
OM:	865	N THR	114	163.006	49.475	62.661	1.00 36.71	L	
MOT	863 864	O PRO	113	164.511	50.988	61.974	1.00 53.16	L	:
MOZ	862 863	CG PRO	113 113	163.223	50.568	61.997	1.00 45.33	L	
MOT	861	CB PRO	113	162.267 163.223	51.018 52.029	59.776 59.220	1.00 32.76	L	
MOT	860	CA PRO	113	162.250	51.316	61.269 59 776	1.00 49.74 1.00 32.76	L L	
ГОМ	859	CD PRO	113	163.153	53.256	60.117	1.00 52.49	L T.	
rom	858	N PRO	113	162.464	52.761	61.325	1.00 51.11	Li T.	
rom	857	O ALA	112	161.447	52.957	63.325	1.00 45.43	L	
rom	856	C ALA	112	162.043	53.476	62.376	1.00 42.23	· L	•
ГОМ	855	CB ALA	112	163.712	55.266	62.887	1.00 43.77	<u>r</u>	
TOM	854	CA ALA	112	162.318	54.977	62.348	1.00 42.20	Ŀ	
rom [°]	853	N ALA	112	161.328	55.685	63.141	1.00 47.00	L	
TOM	852	O ALA	111	159.669	55.363	61.658	1.00 59.98	Ŀ	
rom	851	C ALA	111	160.074	55.815	62.730	1.00 51.95	L	
rom rom	849 850	CA ALA	111	158.123	55.633	64.272	1.00 55.98	L	
rom rom	848 849	N ALA CA ALA	111 111	159.151	56.577	63.661	1.00 59.37	L	
MOT	847	O ASP	110	158.487	57.651	62.932	1.00 55.72	- L	
MOJ	846	C ASP	110	158.022 158.093	58.731 58.882	63.551 64.776	1.00 54.97	L	4
COM	845	OD2 ASP	110	158.641	62.277	60.256	1.00 94.16 1.00 60.38	L L	•
MO	844	OD1 ASP	110	156.656	61.399	60.580	1.00 78.11	L	
MOT	843	CG ASP	110	157.861	61.528	60.889	1.00 84.17	Ŀ	
MOT	842	CB ASP	110	158.395	60.740	62.082	1.00 68.55	L	, v
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ATOM		895	CB	PHE	118		167.260	36.601	58.654	1.00	32.60	, L
ATOM		896	CG	PHE	118		166.589	37.174	59.858	1.00	32.33	. L
MOTA		897	CD1	PHE	118		165.845	38.339	59.761	1.00	32.14	Ŀ
MOTA		898	CD2	PHE	118		166.731	36.572	61.100	1.00	30.97	L
MOTA		899	CE1	PHE	118		165.262	38.902	60.884	1.00	43.45	L
ATOM		900.	CE2	PHE	118		166.148	37.128	62.230	1.00	24.60	L
ATOM		901	CZ	PHE	118		165.411	38.294	62.124	1.00	41.49	L
MOTA	•	902	C	PHE	118		169.339	36.332	57.329	1.00	26.66	Ŀ
ATOM	**	903	0	PHE	118		168.928	36.370	56.170	1.00	29.78	L t :
MOTA		904	N	PRO	119		170.402	35.602	57.685	1.00	34.94	L
ATOM		905	CD	PRO	119		170.999	35.559	59.027	1.00	32.83	$\mathbf{L}_{\mathbf{i}}$
ATOM		906	CA	PRO	119		171.136	34.763	56.734	1.00	37.60	L
MOTA		907	CB	PRO	119		172.400	34.369	57.497	1.00	31.28	L
ATOM		908	CG	PRO	119		172.428	35.261	58.732	1.00	32.18	L
ATOM	,	909	Ċ	PRO	119		170.278	33.551	56.389	1.00	36.29	L
ATOM		910	0	PRO	119		169.297	33.266	57.079	1.00	43.06	L
MOTA		911	N	PRO	120		170.628	32.822	55.321	1.00	33.16	L
ATOM		912	CD	PRO	120		171.752	33.046	54.401	1.00	35.66	L.
ATOM		913	CA	PRO	120		169.838	31.645	54.944	1.00	27.25	L
ATOM		914	CB	PRO	120		170.543	31.110	53.699	1.00	23.84	L
MOTA		915	CG	PRO	120		171.345	32.258	53.186	1.00	47.85	L
MOTA		916	C	PRO	120		169.771	30.597	56.052	1.00	47.51	Ŀ
ATOM		917	0	PRO	120		170.408	30.733	57.097	1.00	61.24	L .
ATOM		918	N	SER	121	*	168.990	29.552	55.812	1.00	46.49	. L
ATOM		919	CA	SER	121		168.836	28.481	56.781	1.00	35.79	L
ATOM		920	CB	SER	121		167.366	28.091	56.908	1.00	39.97	L
MOTA		921	OG	SER	121		166.848	28.512	58.153	1.00	61.95	Ŀ
MOTA	**	922	C	SER	121		169.643	27.264	56.366	1.00	35.14	L
ATOM	,	923	0	SER	121		169.776	26.970	55.178	1.00	54.90	L
ATOM	•	924	N	SER	122	2-	170.190	26.566	57.352	1.00	34.00	L
ATOM		925	CA	SER	122		170.964	25.367	57.078	1.00	43.67	L
ATOM		926	CB	SER	122	ı	171.319	24.661	58.385	1.00	55.34	L
ATOM		927	OG	SER	122		170.845	25.401	59.496	1.00	66.58	L
MOTA	•	928	C .	SER	122		170.038	24.496	56.265	1.00	39.48	L
MOTA		929	0	SER	122		170.345	24.107	55.139	1.00	38.43	L
ATOM		930	N	GLU	123		168.878	24.223	56.850	1.00	39.62	L
MOTA		931	CA	GLU	123		167.865	23.412	56.208	1.00	42.31	. L
ATOM		932	CB	GLU	123		166.569	23.487	57.012	1.00	49.13	L
ATOM		933	CG	GLU	123	•	165.364	22.895	56.294	1.00	85.24	L
ATOM		934	CD	GLU	123		164.237	22.520	57.240	1.00	100.00	T,
ATOM		935		GLU	123		164.458	22.525	58.473	1.00	99.99	. L
ATOM		936	OE2	GLU	123	1	163.127	22.221	56.742	1.00	99.98	L
ATOM		937	C	GLU	123		167.627	23.885	54.774	1.00	34.58	Ŀ
ATOM		938	0	GLU	123		167.599	23.079	53.843		33.93	L
ATOM		939	N	GLN	124		167.467	25.193	54.588		36.30	T.
MOTA		940	CA	GLN	124	•	167.228	25.719	53.254	1.00	21.55	Ŀ
ATOM		941	CB	GLN	124		166.875	27.207	53.289		32.12	L
ATOM	•	942	CG	GLN	124	,	167.075	27.854	51.927	1.00	35.77	L
ATOM	**	943	CD -	GLN	124		166.351	29.160	51.766	1.00	35.92	_ L
ATOM		944	OE1	GLN	124		166.349	29.995	52.669	1.00	37.01	. L
ATOM		945	NE2	GLN	124		165.739	29.355	50.603	1.00	40.10	. L
ATOM	•	946	C	GLN	124		168.441	25.534	52.353		29.80	L
MOTA	4.	947	0 -	GLN	124		168.308	25.269	51.159		40.34	L
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MOTA	948	$\widetilde{oldsymbol{N}}$	LEU	125	r	169.626	25.691	52.921	1.00	29.81		\mathbf{L}
ATOM	949	CA.	LEU	125		170.837	25.538	52.142	1.00	30.50		L
MOTA	950	CB	LEU	125	r	172.047	25.907	52.998	1.00	28.95		L
ATOM	951	CG	LEU	125		172.296	27.418	53.004	1.00	38.05		L
MOTA	952	CD1	LEU	125		173.275	27.794	54.099	1.00	45.58		T,
ATOM	953	CD2	LEU	125		172.814	27.836	51.636	1.00	18.04	•	L
ATOM	954	С	LEU	125		170.952	24.108	51.630	1.00	31.63		Ĺ
ATOM	955	0	LEU	125		171.396	23.873	50.503	1.00	28.04		L
ATOM	956	N	THR	126		170.530	23,156	52.454	1.00	34.33		L
MOTA	957	CA	THR	126		170.570	21.741	52.094	1.00	40.34		L
MOTA	958	CB	THR	126		169.981	20.876	53.226	1.00	47.29		L
MOTA	959	·OG1	THR	126		170.445	21.364	54.490	1.00	38.65		L
ATOM	960	CG2	THR	126		170.397	19.426	53.063	1.00	58.05	٠	L
ATOM	961	С	THR	126		169.806	21.444	50.796	1.00	47.30		L
ATOM	962	0	THR	126		170.142	20.515	50.063	1.00	54.95		L
ATOM	963	N	SER	127		168.779	22.236	50.513	1.00	57.73		L
ATOM	964	CA	SER	127		167.985	22.042	49.308	1.00	63.60		L
ATOM	965	СВ	SER	127		166.551	22.525	49.542	1.00	63.78		L
ATOM	966	OG	SER	127		166.528	23.787	50.186	1.00	64.66		L
MOTA	967	C	SER	127		168.581	22.760	48.096	1.00	67.39		L
ATOM	968	0	SER	127		168.031	22.693	46.994	1.00	73.65	• • ;	L
ATOM	969	N	GLY	128		169.701	23.446	48.303	1.00	60.63		L
ATOM	970	CA	GLY	128		170.350	24.154	47.209	1.00	50.24		L
MOTA	971	C	GLY	128	•	169.838	25.563	46.947	1.00	51.09		L
ATOM	972	0	GLY	128		170.151	26.169	45.917	1.00	49.56		L
MOTA	973	N	GLY	129	**	169.043	26.083	47.877	1.00	48.06		L
ATOM	974	CA	GLY	129		168.507	27.425	47.731	1.00	48.39		L
ATOM	975	C	GLY	129		168.926	28.261	48.919	1.00	45.57		L
ATOM	976	0	GLY	129		169.221	27.719	49.986	1.00	58.83		L
ATOM	977	N	ALA	130		168.964	29.577	48.746	1.00	44.51		L
MOTA	978	CA	ALA	130		169.368	30.467	49.834	1.00	42.67		L
MOTA	979	CB	ALA	130		170.868	30.721	49.766	1.00	41.38	7	L
ATOM	980	C	ALA	130	r	168.612	31.784	49.784	1.00	38.53	:	L
MOTA	981	0	ALA	130	ż	168.661	32.506	48.783	1.00	43.66		L
ATOM	982	N	SER	131		167.923	32.103	50.872	1.00	34.81		L
ATOM	983	CA	SER	131		167.154	33.334	50.936	1.00	28.61		L
ATOM	984	CB	SER	131		165.662	33.019	51.035	1.00	29.28	s. k	L
MOTA	985	OG	SER	131	•	165.165	32.494	4,9.817	1.00	65.36		L
ATOM	986	C.	SER	131		167.568	34.177	52.118	1.00	17.56		L
MOTA	987	. O	SER	131		167.547	33.714	53.259	1.00	23.33	:	L
MOTA	988	N	VAL	132	• •	167.958	35.413	51.842	1.00	21.04		L
MOTA	989	CA	VAL	132		168.353	36.345	52.891	1.00	22.72		L
MOTA	990	CB	VAL	132		169.558	37.211	52.474	1.00	24.09	*	L
MOTA	991	CG1	VAL	132		170.321	37.669	53.711	1.00	37.12		L
MOTA	992	CG2	VAL	132		170.468	36.420	51.535	1.00	26.09	·	L
MOTA	993	C	VAL	132		167.143	37.238	53.115	1.00	27.45		L
MOTA	994	0	VAL	132		166.609	37.836	52.179	1.00	34.77		Ŀ
MOTA	995	N	VAL	133		166.701	37.314	54.360	1.00	21.35		L
MOTA	996	CA	VAL	133		165.532	38.101	54.688	1.00	15.87		L
ATOM	997	CB	VAL	133		164.483	37.235	55.426	1.00	18.41		L
MOTA	998	CG1	VAL	133		163.382	38.111	56.010	1.00	41.56	•	Ŀ
MOTA	999	CG2	VAL	133		163.900	36.211	54.466	1.00	38.08		L
MOTA	1000	C	VAL	133		165.870	39.296	55.548	1.00	10.26		L

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MOTA	1001	0	VÀL	133	166.701	39.222	56.454	1.00 24.39	\mathbf{L}
ATOM	1002	\mathbf{N}	CYS	134	165.206	40.404	55.254	1.00 24.79	Ŀ
MOTA	1003	CA	CYS	134	165.412	41.626	55.999	1.00 33.03	L
MOTA	1004	C	CYS	134	164.070	42.163	56.444	1.00 34.77	L
ATOM	1005	0	CYS	134	163.166	42.338	55.631	1.00 37.02	L
MOTA	1006	CB	CYS	134	166.104	42.660	55.127	1.00 37.32	L
ATOM	1007	SG	CYS	134	166.705	44.083	56.077	1.00 64.48	L
ATOM	1008	N	PHE	135	163.946	42.420	57.737	1.00 28.41	L
ATOM	1009	CA	PHE	135	162.710	42.949	58.296	1.00 35.98	L
ATOM	1010	CB	PHE	135	162.297	42.152	59.536	1.00 23.45	L
ATOM	1011	CG	PHE	135	161.854	40.746	59.244	1.00 41.99	Ľ
ATOM	1012	CD1	PHE	135	160.991	40.472	58.187	1.00 58.79	L
ATOM	1013	CD2	PHE	135	162.280	39.696	60.049	1.00 38.90	L
ATOM	1014	CE1	PHE	135	160.555	39.170	57.939	1.00 56.32	L
ATOM	1015	CE2	PHE	135	161.849	38.391	59.810	1.00 57.18	${f L}$
ATOM	1016	CZ	PHE	135	160.987	38.127	58.753	1.00 46.88	L
ATOM	1017	C	PHE	135	162.880	44.412	58.696	1.00 37.21	L
ATOM	1018	0	PHE	135	163.841	44.773	59.373	1.00 31.75	L
ATOM	1019	N	LEU	136	161.951	45.253	58.264	1.00 38.27	L
ATOM	1020	CA	LEU	136	161.968	46.665	58.622	1.00 33.10	Ŀ
ATOM	1021	CB	LEU	136	162.049	47.531	57.369	1.00 23.62	. L
ATOM	1022	CG	LEU	136	163.303	47.259	56.534	1.00 17.58	· L
ATOM	1023	CD1	LEU	136	163.055	46.103	55.572	1.00 17.79	L
ATOM	1024	CD2	LEU	136	163.686	48.512	55.770	1.00 29.81	L
ATOM	1025	С	LEU	136	160.632	46.839	59.319	1.00 30.65	L
ATOM	1026	O	LEU	136	159.600	47.002	58.673	1.00 30.43	. L
ATOM	1027	N	ASN	137	160.651	46.779	60.643	1.00 35.92	L
ATOM	1028	CA	ASN	137	159,421	46.873	61.400	1.00 43.25	<u> </u>
ATOM	1029	CB .	ASN	137	159.387	45.751	62.433	1.00 42.56	L
ATOM	1030	CG	ASN	137	159.308	44.384	61.793	1.00 30.61	L
ATOM	1031	OD1	ASN	137	159.471	43.356	62.454	1.00 37.72	L
MOTA	1032	ND2	ASN	137	159.057	44.363	60.490	1.00 39.03	L
ATOM	1033	C ·	ASN	137	159.101	48.199	62.075	1.00 40.01	L
MOTA	1034	0	ASN	137	159.975	49.028	62.305	1.00 39.51	L
ATOM	1035	N	ASN	138	157.813	48.362	62.370	1.00 41.07	L
MOTA	1036	CA	ASN	138	157.239	49.526	63.036	1.00 38.43	Ŀ
MOTA	1037	CB	ASN	138	157.227	49,273	64.540	1.00 34.91	L
MOTA	1038	CG	ASN	138	156.667	47.916	64.883	1.00 33.75	$\mathbf{L}_{\mathbf{i}}$
ATOM	1039	OD1	ASN	138	155.592	47.806	65.459	1.00 29.26	Ŀ
MOTA	1040	ND2	ASN	138	157.402	46.864	64.537	1.00 33.12	L
ATOM	1041	C .	ASN	138	157.838	50.898	62.749	1.00 31.73	L
MOTA	1042	0	ASN.	138	158.582	51.447	63.559	1.00 39.37	L
ATOM	1043	N	PHE	139	157.492	51.458	61.599	1.00 32.60	L
MOTA	1044	CA	PHE	139	157.982	52.770	61.227	1.00 34.36	L
ATOM	1045	CB	PHE	139	159.138	52.644	60.237	1.00 37.95	L
MOTA	1046	CG	PHE	139	158.770	51.972	58.946	1.00 21.99	Ŀ
MOTA	1047	CD1	PHE	139	158.295	52.716	57.869	1.00 28.23	Lı
MOTA	1048	CD2	PHE	139	158.941	50.597	58.792	1.00 23.34	L
ATOM	1049	CE1	PHE	139	157.998	52.102	56.651	1.00 22.39	L
ATOM	1050	CE2	PHE	139	158.646	49.969	57.578	1.00 15.56	L
MOTA	1051	CZ	PHE	139	158.175	50.723	56.505	1.00 21.70	L
MOTA	1052	C	PHE	139	156.868	53.626	60.627	1.00 42.27	L
ATOM	1053	0	PHE	139	155.772	53.142	60.350	1.00 50.50	${f L}$
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MOTA	1054	N	TYR	140		157.158	54.906	60.444	1.00 53.69	L
ATOM	1055	CA	TYR	140		156.205	55.847	59.883	1.00 47.40	L
MOTA	1056	CB	TYR	140		155.193	56.266	60.942	1.00 53.56	\mathbf{L}
MOTA	1057	CG	TYR	140		154.002	56.979	60.360	1.00 71.75	L
MOTA	1058	CD1	TYR	140		154.072	58.331	60.029	1.00 76.99	L
MOTA	1059	ÇE1	TYR	140		152.978	58.991	59.471	1.00 91.66	L
MOTA	1060	CD2	TYR	140		152.809	56.301	60.119	1.00 85.47	L
MOTA	1061	CE2	TYR	140	٠	151.712	56.948	59.562	1.00 96.08	· <u>L</u>
MOTA	1062	CZ	TYR	140		151.803	58.293	59.242	1.00 93.77	L
ATOM	1063	OH	TYR	140		150.716	58.946	58.706	1.00 99.99	L
ATOM	1064	Ĉ	TYR	140		156.981	57.065	59.410	1.00 31.82	L
ATOM	1065	0	TYR	140		157.900	57.515	60.088	1.00 34.79	L
ATOM	1066	N	PRO	141		156.631	57.613	58.240	1.00 33.26	$\mathbf{L}_{\mathbf{i}}$
MOTA	1067	CD	PRO	141		157.366	58.764	57.691	1.00 26.57	L
ATOM	1068	CA	PRO	141		155.566	57.178	57.336	1.00 39.66	L
ATOM	1069	CB	PRO	141		155.450	58.321	56.323	1.00 45.22	L
ATOM	1070	CG	PRO	141	**	156.359	59.402	56.804	1.00 34.28	Ŀ
ATOM	1071	C	PRO	141		155.882	55.860	56.651	1.00 32.49	L
ATOM	1072	0	PRO	141		156.913	55.244	56.913	1.00 34.82	L
ATOM	1073	N	LYS	142		154.986	55.438	55.762	1.00 33.41	L
ATOM	1074	CA	LYS	142		155.157	54.191	55.033	1.00 45.13	•
ATOM	1075	CB	LYS	142		153.862	53.816	54.304	1.00 63.72	L
ATOM	1076	CG	LYS	142		152.851	54.942	54.200	1.00 82.02	L
MOTA	1077	CD	LYS	142	•	152.005	54.806	52.943	1.00 86.08	L
ATOM	1078	CE	LYS	142		152.031	56.087	52.114	1.00 97.81	L
ATOM	1079	NZ	LYS	142		153.221	56.173	51.209	1.00100.00	L
ATOM	1080	C	LYS	142		156.290	54.308	54.029	1.00 47.94	— 上
ATOM	1081	0	LYS	142		156.926	53.320	53.679	1.00 60.89	L L
ATOM	1082	N .	ASP	143		156.543	55.523	53.565	1.00 61.49	Ŀ
ATOM	1083	CA	ASP	143		157.605	55.725	52.603	1.00 70.17	 _L
ATOM	1084	CB	ASP	143		157.730	57.203	52.259	1.00 86.10	L L
ATOM	1085	CG	ASP	143	,	156.674	57.656	51.286	1.00 99.99	L L
ATOM	1086	OD1	ASP			155.526	57.891	51.727	1.00 98.78	L
ATOM	1087	OD2	ASP	143		156.992	57.769	50.080	1.00 99.96	L
ATOM	1088	C	ASP	143	•	158.923	55.207	53.148	1.00 62.40	L
ATOM	1089	0	ASP	143		159.344	55.564	54.251	1.00 47.98	L
ATOM	1090	N	ILE	144		159.563		52.363	1.00 59.85	L
ATOM	1091	CA	ILE	144		160.839	53.752	52.722	1.00 51.41	L
ATOM	1092	CB	ILE	144		160.664	*	53.785	1.00 41.53	L
ATOM	1093	CG2	ILE	144		160.074	51.392	53.155	1.00 34.89	L
ATOM	1094		TLE	144	:	162.011	52.320	54.427	1.00 24.47	L
ATOM	1095	CD1	ILE	144	•	161.892	51.470	55.671	1.00 21.68	L
MOTA	1096	CDI	ILE	144	٠	161.441	53.160	51.460	1.00 48.41	L L
MOTA	1097	0	ILE	144		160.719	52.739	50.557	1.00 31.96	L
MOTA	1097	N	ASN	145		162.765	53.142	51.387	1.00 56.85	Ŀ
ATOM	1098	CA	ASN	145		163.447	52.603	50.221	1.00 50.05	Ļ
	1100	CB	ASN	145		164.063	53.730	49.399	1.00 75.48	L L
ATOM						164.104	53.413	47.922	1.00 98.08	L
MOTA	1101 1102	CG OD1	ASN ASN	145 145		163.684	54.221	47.094	1.00 98.00	L
MOTA		ND2	ASN	145 145		163.664	52.231	47.579	1.00 99.99	L
MOTA	1103	G MDS	ASN	145		164.531	51.633	50.650	1.00 52.75	L
ATOM	1104	0		145		165.530	52.024	51.251	1.00 32.73	L
MOTA	1105		ASN			164.324	50.362	50.330	1.00 60.86	L
ATOM	1106	N	VAL	146		104.324	20.302	70.33U	1.00 00.00	اسار

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MOTA	1107	CA	VAL	146		165.283	49.327	50.683	1.00	55.40		L
ATOM	1108	CB	VAL	146	į.	164.572	48.048	51.171	1.00	51.60	•	\mathbf{L}
MOTA	1109	CG1	VAL	146	1 1	165.593	47.066	51.728	1.00	23.45		L
MOTA	1110	CG2	VAL	146		163.545	48.397	52.234	1.00	57.40		L
ATOM	1111	C	VAL	146		166.158	48.975	49.490	1.00	53.23		L
ATOM	1112	0	VAL	146		165.707	48.977	48.341	1.00	69.79	·	L
ATOM	1113	N	LYS	- 147		167.421	48.679	49.775	1.00	49.86		L
MOTA	1114	CA	LYS	147		168.378	48.312	48.746	1.00	42.42		L
MOTA	1115	CB	LYS	147		169.281	49.499	48.413	1.00	47.62		L
ATOM	1116	CG	LYS	147		168.754	50.388	47.302	1.00	79.82		L
ATOM	1117	CD	LYS	147		169.895	51.010	46.512	1.00	86.84	*	L
MOTA	1118	CE	LYS	147		169.939	52.524	46.691	1.00	93.63		$\mathbf{L}_{\mathbf{i}}$
MOTA	1119	NZ	LYS	147		170.983	52.943	47.671	1.00	75.73		L
ATOM	1120	C	LYS	147	•	169.222	47.159	49.265	1.00	35.56		L
ATOM	1121	0	LYS	147		169.545	47.103	50.451	1.00	22.60		L
ATOM	1122	\mathbf{N}	TRP	148		169.566	46.236	48.375	1.00	43.57		L
ATOM	1123	CA	TRP	148		170.386	45.095	48.758	1.00	34.06	,	Ŀ
ATOM	1124	CB	TRP	148		169.782	43.796	48.214	1.00	32.94		L
MOTA	1125	CG	TRP	148		168.782	43.185	49.150	1.00	47.82		L
MOTA	1126	CD2	TRP	148		169.062	42.433	50.338	1.00	46.07		L
ATOM	1127	CE2	TRP	148	*1	167.822	42.096	50.923	1.00	40.42		L
MOTA	1128	CE3	TRP	148		170.243	42.012	50.967	1.00	64.21	ı	${f L}$
MOTA	1129	CD1	TRP	148		167.420	43.270	49.065	1.00	34.71		L
MOTA	1130	NE1	TRP	148	_	166.838	42.621	50.125	1.00	38.06		L
ATOM	1131	CZ2	TRP	148		167.725	41.357	52.109	1.00	15.75	4 7	L
ATOM	1132	CZ3	TRP	148		170.146	41.277	52.148	1.00	72.60		$\mathbf{L}^{\tilde{i}}$
ATOM	1133	CH2	TRP	148		168.894	40.958	52.705	1.00	49.76		L
ATOM	1134	С	TRP	148		171.793	45.269	48.217	1.00	36.36		L
ATOM	1135	0	TRP	148		171.984	45.624	47.055	1.00	34.43		L
ATOM	1136	N	LYS	149		172.784	45.027	49.062	1.00	44.04		L
ATOM	1137	CA	LYS	149		174.157	45.161	48.623	1.00	41.49		L
MOTA	1138	CB	LYS	149		174.820	46.341	49.321	1.00	34.89	,	L
ATOM	1139	CG	LYS	149		175.080	47.515	48.400	1.00	38.34		L
ATOM	1140	CD	LYS	149		174.417	48.774	48.915	1.00	36.55		Ŀ
MOTA	1141	CE	LYS	149		175.294	49.986	48.667	1.00	43.94		L
ATOM	1142	NZ	LYS	149	•	175.270	50.930	49.819	1.00	55.84		L
MOTA	1143	C	LYS	149		174.937	43.893	48.896	1.00	38.62		L
MOTA	1144	0	LYS	149		175.125	43.505	50.045	1.00	42.16		L
ATOM	1145	N	ILE	150		175.372	43.241	47.825	1.00	22.84		L
MOTA	1146	CA	ILE	150		176.157	42.020	47.938	1.00	24.90		L
MOTA	1147	CB	ILE	150		175.675	40.954	46.958	1.00	42.14		L
ATOM	1148	CG2	ILE	150	,	176.371	39.642	47.255	1.00	38.41		L
ATOM	1149	CG1	ILE	150	•	174.159	40.812	47.060	1.00	42.99		L
ATOM	1150	CD1	ILE	150		173.598	39.635	46.309	1.00	32.26		L
ATOM	,1151	C	ILE	150		177.600	42.361	47.614	1.00	23.92		L
MOTA	1152	0	ILE	150		177.975	42.479	46.443	1.00	24.95		L
ATOM	1153		ASP	151		178.404	42.527	48.658	1.00			L
ATOM	1154	ĊA	ASP	151		179.805	42.886	48.488	1.00			L
ATOM	1155	CB	ASP	151		180.507	41.896	47.547	1.00	74.75		L
ATOM	1156	CG	ASP	151		180.844	40.574	48.223	1.00	76.70		L
ATOM	1157	OD1	ASP	151		180.681	40.465	49.460	1.00	79.84		L
ATOM	1158		ASP	151		181.274	39.638	47.508	1.00	56.23		Lı
ATOM	1159	C	ASP	151		179.854	44.300	47.905		70.87		L
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	MOTA	1160	O ,	ASP	151	•	180.483	44.536	46.868	1.00 70.42	L
	MOTA	1161	N	GLY	152		179.172	45.226	48.577	1.00 76.86	· T
٠	ATOM	1162	CA	GLY	152		179.139	46.613	48.139	1.00 67.78	Ŀ
	ATOM	1163	С	GLY	152	"	178.418	46.840	46.824	1.00 70.46	` L
4*	ATOM	1164	0	GLY	152		178.156	47.980	46.438	1.00 79.32	L
	ATOM	1165	N	SER	153		178.098	45.754	46.131	1.00 62.96	. L
	ATOM	1166	CA	SER	153		177.409	45.845	44.856	1.00 60.58	Ŀ
	ATOM	1167	CB	SER	153		177.840	44.693	43.947	1.00 68.60	Ŀ
٠	MOTA	1168	OG	SER	153		178.171	45.160	42.653	1.00 71.40	L
	ATOM.	1169	C	SER	153		175.902	45.800	45.063	1.00 61.38	· L
	ATOM	1170	0	SER	153		175.401	45.044	45.895	1.00 59.28	L
·	ATOM	1171	N	GLU	154		175.183	46.620	44.304	1.00 59,43	L
	ATOM	1172	CA	GLU	154	3	173.731	46.677	44.393	1.00 66.09	L
	ATOM	1173	CB	GLU	154		173.222	47.987	43.793	1.00 81.88	Ŀ
	ATOM	1174	CG	GLU	154		172.299	48.776	44.700	1.00 78.09	L
	ATOM	1175	CD	GLU	154		171.857	50.087	44.079	1.00 85.76	L
	ATOM	1176	OE1	GLU	154		170.891	50.074	43.283	1.00 65.69	L
	MOTA	1177	OE2	GLU	154		172.476	51.131	44.385	1.00 98.75	Ŀ
	ATOM	1178	C	GLU	154		173.123	45.505	43.635	1.00 78.80	L
	ATOM	1179	0	GLU	154		173.476	45.248	42.485	1.00 87.43	L
	MOTA	1180	N	ARG	155	1	172.211	44.791	44.288	1.00 78.61	L
	MOTA	1181	CA	ARG	155		171.552	43.654	43.669	1.00 72.18	L
	ATOM	1182	CB	ARG	155		171.904	42.371	44.411	1.00 57.25	L
	MOTA	1183	CG	ARG	155	•	172.051	41.177	43.500	1.00 53.97	L
	ATOM	1184	CD.	ARG	155		170.868	40.250	43.648	1.00 47.95	I.
	ATOM	1185	NE	ARG	155		170.680	39.401	42.474	1.00 59.26	L
	ATOM	1186	CZ	ARG	155		171.533	38.459	42.084	1.00 47.18	L
	ATOM	1187	NH1		155		172.644	38.239	42.776	1.00 58.65	Ľ
	ATOM	1188	NH2	ARG	155 II		171.272	37.731	41.007	1.00 62.18	· L
	ATOM	1189	C	ARG	155	,	170.049	43.862	43.692	1.00 76.06	L
"	ATOM	1190	0	ARG	155		169.470	44.142	44.741	1.00 79.59	L
	ATOM	1191	:	GLN	156	r	169.426	43.726	42.527	1.00 81.46	Ŀ
	ATOM	1192	CA	GLN	156		167.984	43.913	42.395	1.00 75.51	L
	ATOM	1193	CB	GLN	156		167.702	45.122	41.510	1.00 76.21	
	ATOM	1194	CG	GLN	156		168.779	46.179	41.579	1.00 86.59	L.
	ATOM	1195	CD	GLN	156		168.216	47.575	41.514	1.00 82.98	L
	ATOM	1196	OE1	GLN	156		167.460	47.912	40.597	1.00 74.92	· L
3 11	ATOM	1197	NE2		156		168.579	48.402	42.486	1.00 79.96	L
:	ATOM	1198	C	GLN	156		167.308	42.690	41.799	1.00 75.18	Ľ
1	ATOM	1199	0	GLN	156		166.094	42.663	41.629	1.00 78.45	. Li
	ATOM ·	1200	\mathbf{N}	ASN	157		168.106	41.681	41.485	1.00 69.92	L
	ATOM	1201	CA	ASN	157		167.577	40.460	40.909	1.00 62.62	Ľ
	ATOM	1202	CB	ASN	157	z.	168.587	39.880	39.912	1.00 83.40	L
	ATOM	1203	CG	ASN		:	168.058	38.656	39.189	1.00 96.73	Ŀ
	ATOM	1204	OD1		157		168.142	37.534	39.692	1.00 99.98	L
	ATOM	1205	ND2	:	157		167.509	38.865	38.000	1.00 96.79	L
P	ATOM	1206		ASN	157		167.270	39.440	42.009	1.00 43.07	
	ATOM	1207	0	ASN	157		168.169	38.978	42.711	1.00 51.60	
	ATOM -	1207	N	GLY	158		165.994	39.103	42.166	1.00 37.93	
~	ATOM	1209	CA	GLY	158		165.613	38.126	43.168	1.00 45.50	
	ATOM	1210	CA	GLY	158		165.052	38.719	44.441	1.00 46.88	
	ATOM	1211	0	GLY	158		164.905	38.016	45.438	1.00 46.67	
	ATOM	1212	N	VAL	159		164.730	40.005	44.409	1.00 46.40	
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ATOM	1213	CA	VAL,	159		164.191	40.668	45.582	1.00 48.04	Ŀ
MOTA	1214	CĖ	VAL	159		164.746	42.089	45.707	1.00 46.84	·
MOTA	1215	CG1	VAL	159	,	164.497	42.616	47.106	1.00 49.41	Li,
MOTA	1216	CG2	VAL	159		166.234	42.091	45.398	1.00 31.32	L
MOTA	1217	\mathbf{C}^{\perp}	VAL	159	r	162.668	40.738	45.570	1.00 50.14	L
MOTA	1218	0	VAL	159		162.065	41.111	44.563	1.00 70.43	$\mathbf{L}_{\mathbf{l}}$
MOTA	1219	N	LEU	160		162.060	40.371	46.699	1.00 47.07	L
ATOM	1220	CA	LEU	160		160.606	40.379	46.862	1.00 40.66	L
MOTA	1221	CB	LEU	160		160.060	38.958	46.894	1.00 28.04	L
MOTA	1222	CG	LEU	160		160.148	38.197	45.577	1.00 32.43	L
MOTA	1223	CD1	LEU	160		159.270	36.965	45.669	1.00 37.34	
MOTA	1224	CD2	LEU	160		159.722	39.095	44.413	1.00 7.94	
MOTA	1225	C	LEU	160		160.204	41.077	48.151	1.00 42.42	
MOTA	1226	0	LEU	160	ī	160.474	40.583	49.250	1.00 48.94	
ATOM	1227	N	ASN	161		159.545	42.220	48.011	1.00 40.58	Ŀ
ATOM	1228	CA	ASN	161		159.109	42.996	49.161	1.00 26.69	L
ATOM	1229	CB	ASN	161	•	159.377	44.477	48.917	1.00 24.90	
MOTA	1230	CG	ASN	- 161		160.804	44.746	48.500	1.00 36.23	Ľ -
ATOM	1231	OD1	ASN	161		161.743	44.301	49.153	1.00 55.57	L
MOTA	1232	ND2		161		160.975	45.475	47.407	1.00 47.35	
MOTA	1233	C	ASN	161		157.637	42.792	49.471	1.00 32.25	
ATOM	1234	0	ASN	161		156.850	42.415	48.605	1.00 34.73	. L i
ATOM	1235	N	SER	162	£	157.276	43.052	50.722	1.00 28.82	
ATOM	1236	CA	SER	162		155.908	42.907	51.179	1.00 30.10	
MOTA	1237	CB	SER	162	••	155.655	41.470	51.623	1.00 25.07	L
ATOM	1238	OG -	SER	162	•	154.368	41.341	52.203	1.00 34.98	L
ATOM	1239	C	SER	162		155.687	43.855	52.349	1.00 28.22	
ATOM	1240	0	SER	162		156.542	43.949	53.231	1.00 28.01	**
ATOM	1241	N	TRP	163	-	154.556	44.560	52.346	1.00 44.68	_
ATOM	1242	CA	TRP	163		154.217	45.502	53.413	1.00 47.01	
ATOM	1243	CB	TRP	163		153.977	46.914	52.865	1.00 47.04	
ATOM	1244	CG	TRP	163		155.114	47.542	52.139	1.00 50.28 1.00 47.77	
ATOM	1245	CD2		163	•	155.581	47.209	50.824	1.00 47.77	
ATOM	1246	CE2		163	ı	156.655	48.079	50.529 49.865	1.00 47.30	
ATOM	1247	CE3		163		155.193	46.258 48.573	52.578	1.00 50.04	à
ATOM	1248	CD1		163		155.899 156.828	48.901	51.615	1.00 51.73	•
MOTA	1249	NE1		163		157.349	48.028	49.313	1.00 41.27	
ATOM	1250 1251	CZ2		163 163		155.882	46.206	48.655	1.00 43.64	
ATOM		1		163			47.089	48.391	1.00 31.42	
ATOM	1252	CH2	TRP	163		152.937	45.087	54.111	1.00 47.66	
ATOM	1253	. C	TRP TRP	163		152.056	44.487	53.504	1.00 46.95	
MOTA	1254 1255	O N	THR	164		152.831		55.389	1.00 42.09	
MOTA OTA	1256	· CA	THR	164		151.623	45.119	56.141	1.00 39.34	
ATOM	1257	CB	THR	164		151.927	44.805	57.604	1.00 40.04	
ATOM	1258	OG1		164		152.625	45.911	58.185	1.00 45.73	
ATOM	1259	CG2		164		152.770		57.720	1.00 45.43	
ATOM	1260	C	THR	164	•	150.804	46.400	56.099	1.00 33.70	
ATOM	. 1261	0	THR	164	•	151.268	47.424	55.597	1.00 27.93	
ATOM	1262	N	ASP	165		149.584	46.349	56.620	1.00 29.63	
ATOM	1263	CA		165		148.739	47.533	56.649	1.00 37.94	, , , , , , , , , , , , , , , , , , ,
ATOM	1264	CB	ASP	165		147.261	47.141	56.673	1.00 57.52	
ATOM	1265	CG	ASP	165		146.784			1.00 78.24	
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ATOM	1266	OD1	ASP	165	147.303	47.005	54.302	1.00	92.25	,	L
ATOM	1267	OD2	ASP	165	145.891	45.698	55.364	1.00	85.65		L
ATOM	1268	C	ASP	165	149.078	48.282	57.923	1.00	47.66	N	Lı
ATOM	1269	0 .	ASP	165	149.760	47.746	58.792	1.00	50.50		L
ATOM	1270	N	GLN	166	148.609	49.516	58.030	1.00	47.56		L
ATOM	1271	CA	GLN	166	148.850	50.319	59.220	1.00	42.28	•	\mathbf{L}
ATOM	1272	CB	GLN	166	147.982	51.570	59.185	1.00	44.46		L
ATOM	1273	CG	GLN	166	148.213	52.541	60.320	1.00	29.22		L
ATOM	1274	CD	GLN	166	147.967	53.965	59.885	1.00	17.51		L
ATOM	1275	OE1	GLN	166	146.909	54.283	59.343	1.00	43.27		L
ATOM	1276	NE2	GLN	166	148.949	54.830	60.103	1.00	25.31		L
ATOM	1277	C .	GLN	166	148.462	49.478	60.422	1.00	38.24		L
	1278	0	GLN	166	147.361	48.934	60.465	1.00	28.20		L
ATOM	1279	N	ASP	167	149.361	49.364	61.393	1.00	47.65		L
ATOM	1280	CA	ASP	167	149.072	48.577	62.576	1.00	59.05		L
ATOM	1281	CB	ASP	167	150.200	48.691	63.591	1.00	40.82		L
ATOM	1282	CG	ASP	167	150.022	47.742	64.752	1.00	39.12		L
ATOM	1283	OD1	ASP	167.	149.966	46.517	64.510	1.00	57.63		Ŀ
ATOM	1284		ASP	167	149.927	48.214	65.902	1.00	58.29		L
ATOM	1285	C	ASP	167	147.768	49.040	63.205	1.00	68.64		L
ATOM	1286	0	ASP	167	147.482	50.237	63.274	.1.00	62.87		卫
ATOM	1287	N	SER	168	146.978	48.079	63.658	1.00	81.22		L
ATOM	1288	CA	SER	168	145.695	48.374	64.271	1.00	77.38		${f L}$
ATOM	1289	CB	SER	168	144.865	47.095	64.370	1.00	77.42		L
ATOM	1290	OG	SER	168	145.397	46.080	63.532	1.00	89.64		L
ATOM	1291	C	SER	168	145.839	48.994	65.651	1.00	79.26	r	·L
ATOM	1292	0	SER	168	144.922	49.650	66.139	1.00	85.04		L
ATOM	1293	N	LYS	169	146.990	48.792	66.282	1.00	71.82		L
ATOM	1294	CA	LYS	169	147.210	49.330	67.617	1.00	55.95		L
ATOM	1295	CB	LYS	169	147.785	48.247	68.534	1.00	74.95	•	L
ATOM	1296	CG	LYS	169	147.259	46.849	68.253	1.00	84.17		L
MOTA	1297	CD	LYS	169	148.379	45.938	67.762	1.00	83.79	,	L
ATOM	1298	CE	LYS	169	147.843	44.810	66.885	1.00	85.61		L
ATOM	1299	NZ	LYS	169	148.678	44.588	65.665	1.00	81.34		\mathbf{L}
ATOM	1300	C	LYS	169	148.114	50.556	67.658	1.00	46.88		${f L}$
ATOM	1301	0	LYS	169	147.720	51.614	68.145	1.00	59.39	: ,	L
ATOM	1302	N	ASP ·	170	149.331	50.418	67.142	1.00	40.42		L
ATOM	1303	CA	ASP	170	150.269	51.532	67.164	1.00	32.11		L
ATOM	1304		ASP	170	151.647	51.033	67.620	1.00	37.35		L
ATOM ·	/1305	CG	ASP	170	152.505	50.537	66.479	1.00	58.55		L
ATOM	1306		ASP	170	152.200	49.471	65.909	1.00	65.81		L
ATOM	1307		ASP	170	153.500	51.221	66.162	1.00	76.15		L
ATOM	1308		ASP	170	150.370	52.309	65.856	1.00	34.80		L
MOTA	1309	0 .	ASP	170	151.246	53.159	65.693	1.00	26.65		L
ATOM	1310	N .	SER	171	149.466	52.024	64.927	1.00	29.78	ı	L
ATOM	1311	CA	SER	171	149.429	52.719	63.648	1.00	32.11		Ŀ
ATOM	1312	CB	SER	171	148.876	54.135	63.845		36.91	ž	Ŀ
ATOM	1313	OG	SER	171	147.612	54.105	64.486		87.97		L
ATOM	1314	C	SER	171	150.750	52.809	62.894	1.00			L
ATOM	1315	0 .	SER	171	151.004	53.807	62.223	1.00			Ľ
ATOM	1316	N	THR	172	151.591	51.783	62.993	1.00			L
ATOM	1317	CA	THR	172	152.866	51.788	62.271	1.00			L
ATOM	1318	CB	THR	172	154.046	51.292	63.129		41.47		L
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ATOM	1319	OG1	THR	172	153.590	50.286	64.039	1.00	61.43	L
ATOM	1320	CG2	THR	172	154.686	52.449	63.876	1.00	35.62	L
MOTA	1321	C	THR	172	152.807	50.877	61.058	1.00	25.70	\mathbf{L}
ATOM	1322	,0	THR	172	151.812	50.189	60.826	1.00	23.98	L
ATOM	1323	N	TYR	173	153.892	50.871	60.295	1.00	30.31	L
MOTA	1324	CA	TYR	173	153.985	50.042	59.109	1.00	21.84	L
ATOM	1325	CB	TYR ·	173	154.167	50.911	57.863	1.00	39.03	L
ATOM	1326	CG	TYR	173	152.916	51.668	57.487	1.00	42.99	L
MOTA	1327	CD1	TYR	173	151.794	50.994	57.008	1.00	41.83	L
MOTA	1328	CE1	TYR	173	150.621	51.678	56.709	1.00	59.78	L
MOTA	1329	CD2	TYR	173	152.834	53.050	57.651		48.81	L
MOTA	1330	CE2	TYR	173	151.663	53.745	57.355		38.39	. L
MOTA	1331	CZ	TYR	173	150.560	53.052	56.888	1.00		L
MOTA	1332	OH	TYR	173	149.392	53.723	56.607	,	65.26	. L
MOTA	1333	C	TYR	173	155.160	49.098	59.245		30.15	L
ATOM	1334	0	TYR	173	156.089	49.350	60.009		35.37	L
ATOM	1335	N	SER	174	155.111	48.005	58.505		26.54	L
ATOM	1336	CA	SER	174	156.184	47.035	58.539		25.11	Ŀ
ATOM	1337	CB	SER	174	155.832	45.874	59.467	1.00		Ŀ
ATOM	1338	OG	SER	174	156.004	46.246	60.824		23.41	L
ATOM	1339	C	SER	174	156.394	46.518	57.136	**	28.29	L'
ATOM	1340	0	SER	174	155.475	46.515	56.314		22.73	L
ATOM	1341	N	MET	175	157.614	46.093	56.857		29.61	L
ATOM	1342	CA	MET	175	157.925	45.571	55.552		24.86	L
MOTA	1343	CB	MET	175	158.423	46.693	54.646		16.99 9.33	L. L.
ATOM	1344	CG	MET	175	159.379	46.232 47.595	53.575 52.577	1.00 1.00	36.70	L
ATOM	1345	SD	MET	175	159.949 160.270	46.761	51.036		45.25	L
ATOM	1346	CE	MET	175 175	158.986	44.498	55.686		31.31	L
ATOM	1347	С 0	MET	175	159.800	44.522	56.615		32.20	L
ATOM ATOM	1348 1349	N	MET SER	176	158.947	43.544	54.765		27.89	L
ATOM	1350	CA	SER	176	159.916	42.462	54.737		33.91	L.
ATOM	1351	CB	SER	176	159.263	41.137	55.135		32.59	L
ATOM	1352	OG	SER	176	159.019	40.331	53.997		35.30	L
ATOM	1353	C	SER	176	160.435	42.382	53.312		22.54	Li
ATOM	1354	0	SER	176	159.669	42.497	52:356		28.72	L.
ATOM	1355	N	SER	177	161.743	42.210	53.169	1	21.03	L
ATOM	1356	CA .	SER	177	162.355	42.107	51.856		27.57	L
ATOM	1357	CB	SER	177	163.231	43.320	51.574		32.40	Ŀ
ATOM	1358	QG.	SER	177	163.713	43.272	50.245	1.00	27.68	Ŀ
ATOM	1359	C	SER	177	163.196	40.847	51.802	1.00	22.76	L
ATOM	1360	0	SER	177	164.047	40.621	52.661	1.00	33.72	Ŀ
ATOM	1361	N	THR	178	162.956	40.026	50.788	1.00	18.89	L
ATOM	1362	CA	THR	178	163.687	38.780	50.656	1.00	16.96	L
ATOM	1363	CB	THR	178	162.740	37.580	50.740	1.00	21.10	Ŀ
ATOM	1364	OG1	THR	178	161.938	37.681	51.922	1.00	36.63	L
MOTA	1365	CG2	THR	178	163.533	36.285	50.782	1.00	22.64	Ŀ
ATOM	1366	С	THR	178	164.481	38.675	49.362	1.00	21.04	L
ATOM	1367	0	THR	178	163.949	38.878	48.266	1.00	32.90	L
MOTA	1368	N .	LEU	179	165.764	38.358	49.515	1.00	23.97	L
ATOM	1369	CA	LEU	179	166.679	38.183	48.395	1.00	27.62	L
MOTA	1370	CB	LEU	179	168.000	38.899	48.669	1.00	25.50	Ŀ
ATOM	1371	CG	LEU	179	169.043	38.856	47.557	1.00	25.95	上

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MOTA	1372	CD1	LĖU	179	168.487	39.491	46.291	1.00 44.	04 _. L
ATOM	1373	CD2	LEU	179	170.289	39.591	48.025	1.00 24.	41 L
ATOM	1374	C.	LEU .	179	166.920	36.687	48.293	1.00 22.	54 L
ATOM	1375	0	LEU	179	167.417	36.070	49.236	1.00 16.	26 L
MOTA	1376	N	THR	180	166.558	36.110	47.153	1.00 27.	81 L
ATOM	1377	CA	THR	180	166.699	34.675	46.941	1.00 38.	84 L
ATOM	1378	ÇВ	THR	180	165.343	34.060	46.531	1.00 58.	84 L
ATOM	1379	OG1	THR	180	164.391	34.253	47.585	1.00 69.	01 L
ATOM	1380	CG2	THR	180	165.489	32.571	46.243	1.00 65.	13 L
ATOM	1381	C	THR	180	167.744	34.304	45.893	1.00 38.	32 L
ATOM	1382	0	THR	180	167.658	34.715	44.733	1.00 23.	
MOTA	1383	\mathbf{N}	LEU	181	168.726	33.515	46.318	1.00 50.	
ATOM	1384	CA	LEU	181	169.796	33.059	45.439	1.00 54.	78 L
ATOM	1385	CB	LEU	181	171.118	33.751	45.782	1.00 57.	_
MOTA	1386	CG	LEU	181	171.097	35.239	46.126	1.00 52.	
ATOM	1387	CD1	LEU	181	171.777	35.466	47.468	1.00 64.	
ATOM	1388	CD2	LEU	181	171.800	36.017	45.032	1.00 59.	
MOTA	1389	C	LEU	181	169.978	31.558	45.595	1.00 45.	
MOTA	1390	0	LEU	181	169.250	30.904	46.347	1.00 53.	
ATOM	1391	N	THR	182	170.964	31.021	44.882	1.00 33.	
MOTA	1392	CA	THR	182	171.268	29.601	44.935	1.00 32.	
ATOM	1393	CB	THR	182	171.740	29.086	43.571	1.00 35.	
MOTA	1394	OG1	THR	182	172.994	29.694	43.241	1.00 51.	80 L
ATOM	1395	CG2	THR	182	170.726	29.434	42.497	1.00 10.	
MOTA	1396	C	THR	182	172.371	29.340	45.955	1.00 31.	89 L
MOTA	1397	0	THR	182	173.084	30.256	46.366	1.00 22.	
MOTA	1398	N	LYS	183	172.498	28.086	46.369	1.00 18.	
MOTA	1399	CA	LYS	183	173.521	27.703	47.326	1.00 22.	39 L
MOTA	1400	CB	ĻYS	183	173.539	26.186	47.492	1.00 27.	
MOTA	1401	CG	LYS	183	173.959	25.715	48.868	1.00 21.	
ATOM	1402	CD	LYS	183	174.795	24.443	48.785	1.00 28.	*
MOTA	1403	CE	LYS	183	175.371	24.075	50.148	1.00 65.	
MOTA	1404	NZ	LYS	183	176.860	24.085	50.151	1.00 66.	
MOTA	1405	C	LYS	183	174.847	28.168	46.750	1.00 30.	33. L
MOTA	1406	0	LYS	183	175.732	28.640	47.462	1.00 47.	
MOTA	1407	\mathbf{N}	ASP	184	174.957	28.044	45.436	1.00 33.	23 . L
MOTA	1408	-CA	ASP	184	176.162	28.422	44.729	1.00 32.	28 L
MOTA	1409	CB	ASP	184	176.089	27.931	43.290	1.00 41.	02 · L
MOTA	1410	CG	ASP	184	176.041	26.424	43.199	1.00 63.	
MOTA	1411	OD1	ASP	184	176.516	25.754	44.147	1.00 80.	
MOTA	1412	OD2	ASP	184	175.530	25.907	42.185	1.00 76.	
MOTA	1413	C	ASP	184	176.443	29.910	44.747	1.00 37.	
MOTA	1414	Ο.	ASP	184	177.250	30.379	45.547	1.00 58.	
MOTA	1415	M ·	GLU	185	175.770	30.652	43.873	1.00 33.	24 L
MOTA	1416	CA	GLU	185	175.994	32.088	43.781	1.00 36.	62 L
MOTA	1417	CB	GLU ·	185	175.088	32.691	42.702	1.00 37.	34 L
MOTA	1418	CG	GLU	185	173.899	33.484	43.198	1.00 71.	
MOTA	1419	CD	GLU	185	172.973	33.876	42.058	1.00 78.	07 L
MOTA	1420	OE1	GLU	185	173.399	34.680	41.198	1.00 94.	70 L
MOTA	1421	OE2	GLU	185	171.826	33.378	42.020	1.00 82.	48 L
MOTA	1422	C	GLU	185	175.870	32.849	45.095	1.00 40.	77 L
ATOM	1423	0	GLU	185	176.154	34.039	45.144	1.00 28.	19 L
MOTA	1424	N	TYR	186	175.455	32.171	46.160	1.00 45.	72 L

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32.824 175.357 47.461 1.00 31.13 L CA. TYR 1425 186 MOTA 32.284 MOTA 1426 TYR 174.183 48.271 1.00 29.29 \mathbf{L} CB186 32.396 49.769 174.394 1.00 30.13 L 1427 186 CG TYR MOTA 50.447 33.590 1.00 33.39 L 1428 186 174.131 MOTA CD1 TYR 186 174.314 33.694 51.833 1.00 36.37 1429 CE1 TYR Lı MOTA 31.310 50,509 1.00 34.49 CD2 TYR 186 L 1430 174.850 MOTA 51.893 175.036 31.402 1.00 18.79 L CE2 TYR -186 MOTA 1431 32.594 52.549 L TYR 1432 174.766 1.00 34.18 MOTA CZ186 53.913 L 32.673 1.00 39.71 MOTA 1433 OH TYR 186 174.933 32.530 48:224 1.00 25.69 1434 TYR 186 176.641 L MOTA C 33.358 48.985 1.00 46.65 \mathbb{L} 1435 TYR 186 177.138 MOTA 48.025 1436 GLU 187 177.163 31.327 1.00 33.86 L MOTA \mathbf{N} 30.916 1437 GLU 187 178.380 48.695 1.00 30.31 L CA MOTA L 48.707 1.00 51.43 1438 GLU 187 178.478 29.394 CB MOTA 49.831 1.00 68.32 L GLU 177.688 28.757 MOTA CG. 187 1439 L 177.931 27.269 49.944 1.00 84.34 CDGLU 187 MOTA 1440 26.681 49.000 1.00 72.88 上 178.505 OE1 GLU 187 ATOM 1441 50.980 1.00 92.94 187 26.690 \mathbf{L} ${ t GLU}$ 177.540 OE2 MOTA 1442 L 48.021 1.00 25.34 179.608 31.516 GLU 187 MOTA 1443 C 180.731 L 48.476 1.00 33.80 31.319 GLU 187 ATOM 1444 0 1.00 25.18 32.255 46.937 L 179.393 ATOM 1445 ARG 188 NĿ 32.887 46.238 1.00 28.26 180.504 MOTA 1446 CA ARG 188 44.732 1.00 50.64 \mathbb{L} 180.430 32.583 MOTA 1447 CBARG 188 179.374 43.952 1.00 42.62 \mathbb{L} 33.352 ATOM 1448 CG ARG 188 \mathbb{L} 32.895 42.493 1.00 43.87 1449 CDARG 188 179.332 MOTA 42.378 1.00 93.56 \mathbf{L} 179.213 1450 NE ARG 188 31.440 MOTA L 1.00 99.99 30.659 1451 ARG 180.106 41.779 CZ188 MOTA 41.230 1.00 99.99 L 1452 31.187 NH1 ARG 188 181.192 ATOM 29.345 41.733 1.00 99.98 L 179.918 1453 NH2 ARG 188 ATOM 46.490 1.00 22.65 180.549 34.399 Ŀ .CARG 188 ATOM 1454 45.679 1.00 30.16 181.077 **ARG** 35.160 L 1455 188 ATOM 0 1.00 27.86 34.819 47.626 L 180.001 HIS 189 ATOM 1456 N189 48.023 1.00 21.88 L 1457 179.979 36.223 HIS MOTA CA 189 1.00 40.07 L 1458 HIS 36.871 47.650 CB 178.650 MOTA L 37.107 46.182 1.00 47.15 CG HIS 189 178.480 MOTA 1459 L 178.796 1460 38.171 45.405 1.00 55.79 MOTA CD2 HIS 189 $\mathbf{L}_{\mathbf{I}}$ ND1 HIS 36.185 45.342 1.00 63.86 MOTA 1461 189 177.891 L 1.00 61.64 CE1 HIS 189 177.849 36.672 44.115 MOTA 1462 L 37.876 44.127 MOTA 1463 178.391 1.00 60.31 NE2 HIS 189 36.239 49.531 1.00 29.34 \mathbf{L} HIS 189 180.152 MOTA 1464 C L HIS 189 50.205 1.00 34.87 MOTA 179.750 35.291 1465 · O L 1466 ASN 37:309 50.067 1.00 37.34 190 180.729 MOTA \mathbf{N} 180.961 51.507 ĿĿ ASN 1.00 47.66 1467 190 37.379 MOTA CAL 190 37.855 MOTA 1468 51.795 1.00 68.12 CB ASN 182.388 1.00100.00 L 50.930 183.417 1469 ASN 190 37.167 MOTA CG $\mathbf{L}_{\mathbf{I}}$ MOTA 1470 35.945 50.784 1.00 99.97 OD1 ASN 190 183.407 50.350 \mathbf{L} 1471 MOTA ND2 ASN 190 184.320 37.954 1.00 99.98 Ŀ 1472 ASN 190 180.001 38.252 52.290 1.00 42.97 MOTA C 1473 190 179.383 37.797 53.259 1.00 33.80 \mathbf{L} MOTA ASN 0 51.892 1.00 39.67 L 179.885 39.511 MOTA 1474 SER 191 \mathbf{N} L 40.419 52.614 1.00 30.33 MOTA 1475 SER 191 179.010 CA 1.00 31.09 L 52.801 MOTA 1476 SER 191 179.698 41.774 CB 1.00 59.06 191 179.887 42.056 54.177 Ŀ MOTA 1477 OG SER

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ATOM	1478	C .	SER	191	177.655	40.634	51.967	1.00 34.4	•
ATOM	1479	; O .	SER	191	177.550	40.836	50.753	1.00 48.0	
MOTA	1480	N	TYR	192	176.620	40.574	52.802	1.00 25.0	
MOTA	1481	CA	TYR	192	175.246	40.785	52.361	1.00 22.0	
MOTA	1482	CB	TYR	192 .	174.420	39.517	52.582	1.00 16.5	1
ATOM	1483	CG	TYR	192	174.807	38.444	51.598	1.00 33.83	
MOTA	1484	CD1	TYR	192	174.383	38.511	50.273	1.00 39.7	
ATOM	1485	CE1	TYR	192	174.829	37.592	49.330	1.00 33.7	
MOTA	1486	CD2	TYR	192	175.683	37.417	51.961	1.00 36.7	
ATOM	1487	CE2	TYR	192	176.135	36.492	51.024	1.00 36.4	
MOTA	1488	CZ	TYR	192	175.707	36.587	49.711	1.00 39.5	
MOTA	1489	OH	TYR	192	176.164	35.693	48.766	1.00 31.9	
MOTA	1490	C	TYR	192	174.705	41.961	53.160	1.00 26.5	
MOTA	1491	0	TYR	192	174.749	41.970	54.389	1.00 26.8	
ATOM	1492	N	THR	193	174.205	42.959	52.443	1.00 42.5	
ATOM	1493	CA	THR	193	173.716	44.165	53.086	1.00 49.5° 1.00 59.5°	
ATOM	1494	CB	THR	193	174.621	45.362	52.738	1.00 59.3	
ATOM	1495	OG1	THR	193	175.983	45.025	53.025 53.536	1.00 51.2	
ATOM	1496	CG2	THR	193	174.219	46.592 44.574	52.777	1.00 46.9	
ATOM	1497	C	THR	193	172.285 171.848	44.573	51.621	1.00 57.8	
MOTA	1498	O NT	THR	193	171.578	44.946	53.836	1.00 40.0	
MOTA	1499	N	CYS	194	170.208	45.409	53.738	1.00 39.60	
MOTA	1500	CA	CYS	194 194	170.229	46.894	54.090	1.00 50.9	
ATOM	1501	C .	CYS CYS	194	170.419	47.263	55.253	1.00 50.4	
ATOM	1502	O ·			169.326	44.652	54.719	1.00 56.3	
MOTA	1503 1504	CB SG	CYS CYS	194	167.606	45.219	54.662	1.00 57.5	
ATOM ATOM	1504	N	GLU	195	170.039	47.734	53.080	1.00 62.9	
ATOM TO	1505	CA	GLU	195	170.066	49.182	53.262	1.00 56.6	
ATOM	1507	CB.	GLU	195	171.006	49.802	52.231	1.00 67.8	
ATOM	1508	CG	GLU	195	171.618	51.121	52.650	1.00 75.8	
ATOM	1509	CD	GLU	•	172.492	51.711	51.560	1.00 66.0	8 L
ATOM	1510	OE1	GLU	. 195	171.941	52.170	50.533	1.00 83.9	1 L
ATOM	1511	OE2	GLU	195	173.731	51.710	51.731	1.00 69.6	3 L
ATOM	1512	C	GLU	195	168.689	49.812	53.128	1.00 41.9	б L
ATOM	1513	0	GLU	195	167.926	49.466	52.224	1.00 46.9	3 L
ATOM	1514	N	ALA	196	168.381	50.755	54.014	1.00 39.4	8 L
ATOM	1515	CA	ALA	196	167.085	51.419	53.983	1.00 55.4	4 L
MOTA	1516	CB	ALA	196	166.114	50.674	54.880	1.00 62.9	5 L
MOTA	1517	С	ALA	196	167.111	52.897	54.375	1.00 56.7	8 _. L
MOTA	1518	0	ALA	196	167.572	53.254	55.460	1.00 57.4	6 Ь
ATOM	1519	N	THR	197	166.606	53.748	53.484	1.00 59.2	6 L
ATOM	1520	CA	THR	197	166.532	55.186	53.738	1.00 71.5	0 L
ATOM	1521	CB	THR	197	166.971	56.023	52.502	1.00 77.1	3 L
ATOM	1522	OG1	THR	197	166.548	55.374	51.295	1.00 83.3	7 L
ATOM	1523	CG2	THR	197	168.486	56.185	52.483	1.00 62.6	2 L
MOTA	1524	C	THR	197	165.086	55.538	54.086	1.00 73.2	
MOTA	1525	0	THR	197	164.155	55.182	53.362	1.00 73.2	
ATOM	1526	N	HIS	198	164.901	56.233	55.200	1.00 66.2	
ATOM	1527	CA	HIS	198	163.570	56.617	55.655	1.00 65.2	
MOTA	1528	CB	HIS	198	163.203	55.777	56.889	1.00 59.6	
ATOM	1529	CG	HIS	198	161.802	55.976	57.386	1.00 50.0	
ATOM -	1530	CD2	HIS	198	161.333	56.281	58.619	1.00 10.4	6 L

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	MOTA	1531	ND1	HIS	198		160.691	55.811	56.586	1.00 23.72	L
	ATOM	1532	CE1	HIS	198	•	159.601	56.009	57.306	1.00 8.26	L
	ATOM	·1533	NE2	HIS	198		159.962	56.295	58.545	1.00 26.12	L
	ATOM	1534	C	HIS	198		163.611	58.101	56.001	1.00 65.53	$\mathbf{L}_{\mathbf{l}}$
	ATOM	1535	0	HIS	198	•	164.642	58.601	56.446	1.00 44.38	L
	MOTA	1536	N	LYS	199		162.501	58.804	55.776	1.00 69.60	L
	ATOM	1537	CA	LYS	199		162.407	60.235	56.078	1.00 62.83	L
	ATOM	1538	СВ	LYS	199		160.940	60.665	56.214	1.00 59.10	L
	ATOM	1539	CG	LYS	199		160.168	60.725	54.908	1.00 66.79	L
	ATOM	1540	CD	LYS	199		159.541	59.376	54.566	1.00 77.11	L
	ATOM	1541	CE	LYS	199		160.458	58.543	53.670	1.00 66.29	L
	ATOM	1542	NZ	LYS	199		160.372	58.922	52.226	1.00 71.28	Ŀ
	ATOM	1543	С	LYS	199		163.100	60.459	57.409	1.00 54.65	L
	ATOM	1544	0	LYS	199		163.853	61.418	57.596	1.00 52.78	L.
	ATOM	1545	Ň	THR	200		162.823	59.538	58.322	1.00 59.05	L
	ATOM	1546	CA	THR	200		163.361	59.542	59.668	1.00 72.79	L
	ATOM	1547	CB	THR	200		162.896	58.262	60.404	1.00 72.74	
	ATOM	1548	OG1	THR	200		162.485	58.594	61.732	1.00 81.55	. <u>L</u>
	ATOM	1549	CG2	THR	200		164.002	57.222	60.439	1.00 67.03	L
	ATOM	1550	C	THR	200	•	164.890	59.648	59.712	1.00 77.51	L
	MOTA	1551	0	THR	200		165.479	59.774	60.785	1.00 76.37	L
	ATOM	1552	N	SER	201		165.536	59.607	58.550	1.00 82.04	L
	ATOM	1553	CA	SER	201		166.991	59.696	58.521	1.00 77.00	L
	ATOM	1554	CB	SER	201		167.599	58.411	59.082	1.00 70.20	L
	ATOM	1555	OG	SER	201		168.828	58.678	59.728	1.00 48.40	L
	ATOM	1556	C	SER	201		167.583	59.967	57.145	1.00 75.86	L
	ATOM	1557	. 0	SER	201		167.126	59.436	56.129	1.00 78.72	Ŀ
	ATOM	1558	N	THR	202		168.617	60.802	57.128	1.00 79.38	L
	ATOM	1559	CA	THR	202		169.317	61.144	55.897	1.00 85.40	L
	ATOM	1560	CB	THR	202		169.864	62.586	55.942	1.00 82.98	L
	ATOM	1561	OG1	THR	202	1	170.536	62.807	57.190	1.00 58.44	- L
	ATOM	1562	CG2	THR	202		168.725	63.591	55.800	1.00 81.93	L
	ATOM	1563	C	THR	202		170.481	60.165	55.752	1.00 87.12	L
	ATOM	1564	0	THR	202		171.106	60.069	54.697	1.00 90.15	L
	MOTA	1565	N	SER	203		170.757	59.442	56.835	1.00 85.15	Ŀ
	ATOM	1566	CA	SER	203	•	171.826	58.452	56.866	1.00 85.74	L
	ATOM	1567	CB	SER	203	۱.,	172.589	58.538	58.194	1.00 91.67	L
:	ATOM	1568	OG -	SER	203		172.049	59.540	59.041	1.00 86.93	L
	MOTA	1569	С	SER	203		171.203	57.069	56.719	1.00 87.87	L
	ATOM	1570	0	SER	203	**	170.682	56.508	57.686	1.00 84.65	L
	ATOM	1571	N	PRO	204		171.244	56.501	55.502	1.00 89.56	L
•	ATOM	1572	CD	PRO	204		171.858	57.072	54.292	1.00 93.06	L
	MOTA	1573	CA	PRO	204		170.672	55.176	55.244	1.00 82.77	L
	MOTA	1574	CB	PRO	204		171.269	54.772	53.888	1.00 81.38	L
:	ATOM	1575	CG	PRO	204		172.262	55.855	53.525	1.00 78.75	L
	MOTA	1576	C ·	PRO	204		171.002	54.167	56.335	1.00 76.12	L
	MOTA	1577	0	PRO	204		172.169	53.960	56.656	1.00 79.62	Ŀ
	MOTA	1578	N	ILE	205		169.971	53.557	56.911	1.00 69.79	L
	ATOM	1579	CA	ILE	205		170.172	52.556	57.953	1.00 59.52	L
	MOTA	1580	CB	ILE	205		168.862	52.224	58.675.	1.00 59.30	L
•	MOTA	1581	CG2	ILE	205		169.124	51.192	59.763	1.00 62.73	L
	ATOM	1582	CG1	ILE	205		168.264	53.503	59.263	1.00 51.85	L
	ATOM	1583	CD1	ILE	205		166.912	53.310	59.921	1.00 48.97	L
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ATOM	. 1584	C	ILE	205	170.711	51.294	57.294	1.00 58.53	Ŀ
ATOM	1585	0	ILE	205	170.225	50.873	56.241	1.00 60.90	L
ATOM	1586	N	VAL ·	206	171.719	50.691	57.918	1.00 53.53	,L [:]
MOTA	1587	CA	VAL	206	172.332	49.498	57.356	1.00 41.22	\mathbf{L}
ATOM	1588	CB	VAL	206	173.739	49.825	56.810	1.00 18.34	L
ATOM	1589	CG1	VAL	206	174.486	48.548	56.467	1.00 13.15	L
ATOM	1590	CG2	VAL	206	173.618	50.706	55.580	1.00 13.65	Ļ
ATOM	1591	C	VAL	206	172.442	48.336	58.331	1.00 44.96	L
ATOM	1592	0	VAL	206	172.747	48.517	59.509	1.00 44.72	L
ATOM	1593	N	LYS	207	172.180	47.137	57.818	1.00 51.44	${f L}$
ATOM	1594	CA	LYS	207	172.269	45.915	58.598	1.00 52.57	L
ATOM	1595	CB	LYS	207	170.882	45.438	59.020	1.00 54.70	L
ATOM	1596	CG	LYS	207	170.800	45.038	60.479	1.00 47.68	L
ATOM	1597	CD	LYS	207.	171.141	46.206	61.394	1.00 42.68	L
ATOM	1598	CE	LYS	207	170.477	46.060	62.758	1.00 53.93	L
ATOM	1599	NZ	LYS	207	170.763	44.740	63.395	1.00 56.72	Ŀ
ATOM	1600	C	LYS	207	172.906	44.900	57.671	1.00 51.25	L
ATOM	1601	0	LYS	207	172.357	44.592	56.610	1.00 57.87	Ŀ
ATOM	1602	N	SER	208	174.072	44.396	58.059	1.00 48.56	, L i
ATOM	1603	CA	SER	208	174.780	43.429	57.230	1.00 44.28	L
ATOM	1604	CB	SER	208	175.956	44.095	56.525	1.00 43.06	L
ATOM	1605	0G	SER	208	175.511	45.119	55.659	1.00 64.64	L
ATOM	1606	C	SER	208	175.301	42.236	58.003	1.00 46.92	L
ATOM	1607	0 .	SER	208	175.121	42.129	59.221	1.00 49.18	. L
ATOM	1608	N	PHE	209	175.950	41.342	57.269	1.00 47.47	L
ATOM	1609	CA	PHE	209	176.539	40.152	57.850	1.00 48.36	L
ATOM	1610	CB	PHE	209	175.443	39.170	58.296	1.00 58.47	, L
ATOM	1611	CG	PHE	209	174.804	38.414	57.168	1.00 68.93	L
ATOM	1612	CD1	PHE	209	173.734	38.960	56.471	1.00 77.87	L
ATOM	1613	CD2	PHE	209	175.280	37.161	56.793	1.00 73.00	· L
ATOM	1614	CE1	PHE	209	173.148	38.270	55.411	1.00 71.56	\mathbf{r}
ATOM	1615	CE2	PHE	209	174.703	36.461	55.736	1.00 64.61	L
ATOM	1616	CZ	PHE	209	173.633	37.017	55.043	1.00 71.74	L ·
ATOM	1617	С	PHE	209	177.481	39.498	56.851	1.00 44.99	${f r}$
ATOM	1618	0	PHE	209	177.336	39.658	55.637	1.00 35.92	L
ATOM	1619	N	ASN	210	178.463	38.782	57.384	1.00 56.65	L
ATOM	1620	CA	ASN	210	179.444	38.079	56.572	1.00 60.29	L
ATOM	1621	CB	ASN	210	180.853	38.402	57.064	1.00 70.34	. · L
ATOM	1622	CG	ASN	210	181.925	37.920	56.112	1.00100.00	L
ATOM	1623		ASN	210	182.386	38.670	55.250	1.00 99.98	${f L}$
	1624		ASN	210	182.328	36.658	56.258	1.00100.00	${f L}$
ATOM	1625	C	ASN	210	179.165	36.592	56.741	1.00 63.50	. L
ATOM	1626	·	ASN	210	178.624	36.183	57.763	1.00 79.33	L
	1627	N	ARG	211	179.524	35.780	55.756	1.00 60.96	L
ATOM	1628	CA	ARG	211	179.284	34.350	55.872	1.00 67.53	L
ATOM	1629	CB	ARG	211	179.672	33.644	54.576	1.00 53.17	L
ATOM	1630	CG	ARG	211	178.475	33.141	53.792	1.00 46.30	L
ATOM	1631	CD	ARG	211	178.602	33.466	52.320	1.00 24.02	\mathbf{L}
ATOM	1632	NE .	ARG	211	179.366	32.449	51.606	1.00 24.23	L
ATOM	1633	CZ	ARG	211	180.693	32.431	51.527	1.00 46.60	·
ATOM	1634	NH1	ARG	211	181.411	33.377	52.118	1.00 74.04	Ŀ
ATOM	1635	NH2	ARG	211	181.307	31.466	50.863	1.00 58.03	L
ATOM	1636	C	ARG	211	180.041	33.746	57.060	1.00 78.01	L
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MOTA	1637	0	ARG	211		181.277	33.714	57.080	1.00 62.45	${f L}$
MOTA	1638	$N \rightarrow$	ASN	212		179.264	33.284	58.046	1.00 96.28	L
MOTA	1639	CA	ASN	212	1	179.747	32.661	59.288	1.00 99.99	Ţ
MOTA	1640	CB	ASN	212		181.065	31.915	59.055	1.00 99.98	${f L}$
MOTA	1641	CG	ASN	212		181.130	30.602	59.816	1.00100.00	L
MOTA	1642	OD1	ASN	212		180.343	30.360	60.738	1.00 94.94	· L
MOTA	.1643	ND2	ASN	212		182.070	29.743	59.434	1.00 99.99	L
ATOM	1644	C	ASN	212		179.918	33.640	60.455	1.00 99.98	$\mathbf L$
ATOM	1645	0	ASN	212		180.791	34.533	60.359	1.00 99.99	L
ATOM	1646	\mathbf{TO}	ASN	212		181.064	34.157	61.055	1.00 99.99	$oldsymbol{T}$
ATOM	1647	CB	VAL	2	•	121.621	36.267	64.620	1.00 37.38	H
MOTA	1648	CG1	VAL	.2		120.401	36.241	65.515	1.00 27.71	H
MOTA	1649	CG2	VAL	2		122.281	37.627	64.680	1.00 34.18	H
MOTA	1650	C	VAL	· 2		123.855	35.223	64.193	1.00 42.92	H
MOTA	1651	Ο,	VAL	2		124.332	36.300	63.840	1.00 42.57	H
MOTA	1652	N	VAL	2		122.979	35.304	66.494	1.00 47.65	H
MOTA	1653	CA	VAL	2	,	122.610	35.160	65.057	1.00 44.59	H
MOTA	1654	N	GLN	3		124.382	34.056	63.852	1.00 45.14	H
ATOM	1655	CA	GLN	3		125.594	33.990	63.047	1.00 47.76	H
MOTA	1656	CB	GLN	3		126.585	33.018	63.684	1.00 47.79	H
ATOM	1657	CG	GLN	3		128.013	33.216	63.226	1.00 70.50	H
ATOM	1658	CD	GLN	. 3		128.654	31.926	62.768	1.00 77.13	H
ATOM	1659	OE1	GLN	3	£.	128.477	30.879	63.392	1.00 89.69	H
ATOM	1660	NE2	GLN	, 3		129.403	31.990	61.671	1.00 74.80	H
MOTA	1661	C	GLN	3		125.324	33.576	61.605	1.00 43.77	H
ATOM	1662	0	GLN	. 3		124.223	33.144	61.264	1.00 28.11	H
MOTA	1663	N	LEU	4		126.341	33.721	60.761	1.00 43.76	H
ATOM	1664	CA	LEU	4	·	126.231	33.358	59.356	1.00 47.78	H:
ATOM.	1665	CB	LEU	4		126.061	34.620	58.502	1.00 41.23	H
ATOM	1666	CG	LEU	4		125.041	34.700	57.351	1.00 30.41	H
MOTA	1667	CD1		4	÷	124.005	33.592	57.439	1.00 25.02	Н
MOTA	1668	CD2		4		124.353	36.059	57.404	1.00 18.34 1.00 47.69	H
ATOM	1669	C	LEU	4	•	127.499	32.620	58.945 58.524	1.00 47.69 1.00 52.13	H
MOTA	1670	0	LEU	4		128.468 127.500	33.245 31.296	59.081	1.00 32.15	H
MOTA	1671	N	GLN	5 5		127.500	30.500	58.706	1.00 47.49	H
MOTA	1672	CA	GLN	5 5		128.591	29.109	59.335	1.00 47.13	
MOTA	1673	CB CG	GLN	· 5		129.142		60.747	1.00 41.56	H
MOTA	1674 1675	CD	GLN	5		128.328	28.100	61.633	1.00 64.06	H
ATOM ATOM	1676	OE1		5	•	128.475	26.874	61.573	1.00 60.56	H
ATOM	1677	NE2	GLN	5	*	127.459	28.681	62.459	1.00 60.41	H
ATOM -	1678	C	GLN	5		128.764	30.379	57.187	1.00 36.59	$^{\cdot}$ H
ATOM	1679	0	GLN	5		127.760	30.146	56.519	1.00 31.08	H
ATOM	1680	N	GLN	6		129.978	30.531	56.659	1.00 35.83	H
ATOM	1681	CA	GLN	6	•	130.214	30.460	55.220	1.00 33.41	H
ATOM	1682	CB	GLN	6		130.697	31.824	54.715	1.00 15.61	H
ATOM	1683	CG.	GLN	. 6		130.089	32.252	53.377	1.00 48.11	H
ATOM	1684	CD	GLN	6		130.061	33.762	53.195	1.00 44.23	H
ATOM	1685	OE1	GLN	6		129.429	34.480	53.971	1.00 44.77	H
ATOM	1686	NE2		. 6		130.750	34.251	52.164	1.00 43.09	H
ATOM	1687	C	GLN	. 6		131.230	29.393	54.818	1.00 39.29	H
ATOM	1688	0	GLN	6		131.746	28.655	55.659	1.00 47.11	H
MOTA	1689	N	SER	7		131.492	29.318	53.514	1.00 52.14	H
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ATOM	,1690	CA	SER	7.	. ,	132.464	28.402	52.913	1.00 45	.28	•	H
MOTA	1691	CB	SER	·. 7		133.561	28.037	53.913	1.00 30	.02	• •	H
MOTA	1692	OG	SER	7		134.775	27.764	53.240	1.00 36	.01	ı	H·
ATOM	1693	С	SER	7		131.963	27.125	52.255 ·	1.00 53	.29		H
MOTA	1694	0	SER	7	"	130.825	26.691	52.435	1.00 41	.78	2	H
MOTA	1695	M.	GLY	. 8		132.873	26.546	51.478	1.00 74	.11		H
MOTA	1696	CA	GLY	. 8		132.656	25.313	50.744	1.00 86	.06		H
ATOM	1697	C	GLY	8		133.987	25.088	50.046	1.00 96	.74		H
MOTA	1698	0	GLY	8		135.032	25.207	50.691	1.00 99	.99		H
MOTA	1699	N	PRO	9		133.999	24.757	48.739	1.00 99	.99		H
ATOM	1700	CD	PRO	· 9	Ť	132.851	24.529	47.850	1.00 99	.99		H
ATOM	1701	CA	PRO	9		135.283	24.547	48.047	1.00 95	.17		H
ATOM	1702	CB	PRO	. 9		134.873	23.925	46.702	1.00 99	.99		H
MOTA	1703	CG	PRO	9		133.404	23.557	46.852	1.00 99	.98		H
MOTA	1704	C	PRO	9		136.019	25.882	47.872	1.00 83	.28		H
MOTA	1705	0	PRO	9		135.387	26.937	47.793	1.00 73	.84		H
MOTA	1706	N	GLU	10		137.349	25.847	47.811	1.00 73	.05		H
MOTA	1707	CA	GLU	10		138.109	27.087	47.672	1.00 56	.11		H
MOTA	1708	CB	GLU	10		139.003	27.279	48.898	1.00 43	.53		H
MOTA	1709	CG	GLU	10		138.487	26.554	50.136	1.00 30	.69		Η
MOTA	1710	CD	GLU	10		137.988	27.497	51.217	1.00 42	.43		H
MOTA	1711	OE1	GLU	10		138.782	28.352	51.678	1.00 16	.81		H
MOTA	1712	OE2	GLU	10		136.803	27.374	51.612	1.00 22	.46		H
ATOM	1713	C	GLU	10		138.939	27.223	46.393	1.00 47	.28		H
MOTA	1714	0	GLU	10	1	139.302	28.336	46.017	1.00 48	.73		H
MOTA	1715	N	LEU	11		139.239	26.106	45.730	1.00 37	.54	:	H
MOTA	1716	CA	LEU	11		140.012	26.137	44.486	1.00 30	.14		H
ATOM	1717	CB.	LEU	11		141.398	25.517	44.676	1.00 20	.14		H
MOTA	1718	CG	LEU	11		142.591	26.256	44.045	1.00 23	.62		H
ATOM	1719	CD1	LEU	11		143.477	25.265	43.309	1.00 18	.85		H
ATOM	1720	CD2	LEU	11		142.110	27.357	43.100	1.00 23	.67		H
MOTA	1721	C	LEU	11	•	139.306	25.400	43.357	1.00 44	. 95		H
ATOM	1722	• 0	LEU	11		138.867	24.257	43.519	1.00 54	.63		H ·
MOTA	1723	N	VAL	12	•	139.210	26.057	42.207	1.00 41	.04		H
MOTA	1724	CA	VAL	12		138.564	25.466	41.042	1.00 44	.92		H
MOTA	1725	CB	VAL.	12		137.198	26.116	40.760	1.00 55	.40		H
MOTA	1726	CG1	VAL	12		136.166	25.600	41.736	1.00 60	.33		H
MOTA	1727	CG2	VAL	12		137.324	27.631	40.849	1.00 67	.40	·	H
MOTA	1728	C	VAL	12		139.428	25.687	39.824	1.00 38	.99		H
ATOM	1729	O	VAL	12	:	140.065	26.727	39.702	1.00 23	.16	:	H
ATOM ·	1730	\mathbf{N}	LYS	13	1	139.451	24.705	38.928	1.00 56	.02	·	H
MOTA	1731	CA	LYS	13		140.230	24.817	37.701	1.00 61	.99		H
ATOM	1732	CB	LYS	13		140.577	23.430	37.154	1.00 47	.53	r.	H
MOTA	1733	CG	LYS	13		142.054	23.066	37.259	1.00 29	.92		H
MOTA	1734	CD	LYS	13		142.364	21.831	36.416	1.00 39	.21		H
MOTA	1735	CE	LYS	13		143.629	22.007	35.596	1.00 40	.05		H
MOTA	1736	NZ .	LYS	13		144.804	21.337	36.230	1.00 30	.64		H
ATOM	1737	C	LYS	13	•	139.365	25.595	36.706	1.00 60	.22		H
MOTA	1738	0	LYS	13		138.184	25.287	36.513	1.00 48	.99		H
ATOM	1739	N	PRO	14		139.951	26.619	36.066	1.00 55	.96		H
MOTA	1740	CD	PRO	14		141.359	27.003	36.236	1.00 55	.17		H
MOTA	1741	CA	PRO	14		139.270	27.477	35.091	1.00 63	.02		H
MOTA	1742	CB ·	PRO	14		140.412	28.234	34.404	1.00 59	.73		H
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ATOM	1743	CG	PRO	14	¢	141.685	27.633	34.929	1.00	60.43	,	H
ATOM	1744	C ·	PRO	14		138.356	26.766	34.096	1.00	61.60		H
ATOM	1745	0	PRO	14		138.802	25.957	33.275	1.00	63.48		H
ATOM	1746	N	GLY	15		137.069	27.093	34.185	1.00	55.03		H
ATOM	1747	CA	GLY	15		136.077	26.503	33.307	1.00	55.23		H
ATOM	1748	С	GLY	15		134.961	25.815	34.071	1.00	49.69		H
ATOM	1749	0	GĹY	. 15		133.800	25.865	33.670	1.00	45.93		H
ATOM	1750	N	THR	16		135.304	25.176	35.182	1.00	46.88		H
ATOM	1751	CA	THR	16		134.303	24.480	35.969	1.00	46.72		H
ATOM	1752	CB	THR	16		134.946	23.549	36.992	1.00	53.32		H
ATOM	1753	OG1	THR	16		135.914	24.275	37.758	1.00	63.69		H
ATOM	1754	CG2	THR	16		135.615	22.387	36.286	1.00	61.76		H
MOTA	1755	C	THR	16		133.361	25.415	36.700	.1.00	42.84		H
ATOM	1756	Ο.	THR	16		133.391	26.626	36.505	1.00	35.33		H
ATOM	1757	N	SER	17		132.535	24.829	37.559	1.00	46.34		H
ATOM	1758	CA	SER	17	**	131.543	25.570	38.320	1.00	44.29		\mathbf{H}
ATOM	1759	CB	SER	17		130.190	25.458	37.621	1.00	43.09		H
MOTA	1760	OG	SER	17		130.349	25.482	36.211	1.00	37.03		\mathbf{H}
ATOM	1761	C	SER	17	ı	131.408	25.051	39.742	1.00	45.39		H
MOTA	1762	0	SER	17		131.124	23.872	39.956	1.00	51.18		\mathbf{H}
MOTA	1763	N	VAL	18		131.599	25.938	40.713	1.00	43.96	٠	H
ATOM	1764	CA	VAL	18		131.483	25.564	42.119	1.00	45.50		\mathbf{H}
ATOM	1765	CB	VAL	18		132.723	25.989	42.932	1.00	47.04	•	H
ATOM	1766	CG1	VAL	18		132.979	27.469	42.756	1.00	45.76		H
ATOM	1767	CG2	VAL	18		132.513	25.665	44.400	1.00	36.17		\mathbf{H}_{\cdot}
ATOM	1768	C	VAL	18		130.257	26.218	42.742	1.00	46.62		H
ATOM	1769	0	VAL	18		129.772	27.240	42.258	1.00	24.82		H
ATOM	1770	N	ARG	19		129.758	25.610	43.813	1.00	53.11		\mathbf{H}
ATOM	1771	CA	ARG	19	•	128.589	26.122	44.518	1.00	58.98		H
MOTA	1772	CB	ARG '	19		127.414	25.157	44.354	1.00	48.17		H
ATOM	1773	CG	ARG	19		126.252	25.443	45.280	1.00	32.81		H
ATOM	1774	CD	ARG	19		125.479	24.167	45.605	1.00	61.51	•	H
MOTA	1775	NE	ARG	19	1	126.212	23.302	46.530	1.00	70.76	•	H
ATOM	1776	CZ	ARG	19		125.661	22.352	47.283	1.00	68.17		H
MOTA	1777	NH1	ARG	19.		124.353	22.124	47.232	1.00	41.10		H
MOTA	1778	NH2	ARG	19		126.428	21.625	48.090	1.00	47.54		H
ATOM	1779	C	ARG	19		128.912	26.282	46.000	1.00	57.70	•	H
MOTA	1780	0 ,	ARG	19		129.050	25.294	46.716	1.00	66.45		\mathbf{H}
MOTA	1781	N	ILE	20		129.043	27.523	46.456	1.00	53.34		H
ATOM .	1782	CA	ILE	20	**:	129.345	27.780	47.860	1.00	52.34	;	\mathbf{H}
MOTA	1783	CB	ILE	, 20		130.052	29.137	48.067	1.00	45.51		H
MOTA	1784	CG2	ILE	20	*	131.474	29.053	47.565	1.00	47.12		H
MOTA	1785	CG1	ILE	20		129.280	30.243	47.353	1.00	39.21		H
MOTA	1786	CD1	ILE	20		129.929	31.606	47.466	1.00	37.76	s.	H
ATOM	1787	C	ILE	20		128.059	27.800	48.666	1.00			H
MOTA	1788	0	ILE	20		126.960	27.764	48.113	1.00			H
MOTA	1789	N	SER	21		128.208	27.860	49.981	1.00			H
MOTA	1790	CA	SER	21		127.058	27.892	50.863	1.00			H
MOTA	1791	CB	SER	21		126.810	26.503	51.468	1.00		•	H
MOTA	1792	OG	SER	21		127.562	26.314	52.654	1.00			H
ATOM	1793	C	SER	21		127.260	28.917	51.968	1.00			H
ATOM	1794	0	SER	21		128.288	29.599	52.026	1.00			H
MOTA	1795	N	CYS	22		126.262	29.013	52.839	1.00	69.21	•	H
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ATOM	1796	CA	CYS	22	126.263	29.940	53.963	1.00 61.84	\mathbf{H}_{i}
MOTA	1797	C	CYS	22	124.996	29.635	54.745	1.00 52.88	H
MOTA	1798	0	CYS	22	123.890	29.845	54.249	1.00 52.20	, H
MOTA	1799	CB	CYS	22	126.233	31.379	53.461	1.00 52.16	H
MOTA	1800	SG	CYS	22	125.483	32.535	54.637	1.00 54.59	H
MOTA	1801	N	GLU	23	125.154	29.147	55.968	1.00 40.82	H
MOTA	1802	CA	GLU	23 .	123.998	28.783	56.767	1.00 43.24	H
MOTA	1803	CB	GLU	23	124.140	27.339	57.230	1.00 55.82	H
MOTA	1804	CG	GLU	23	125.578	26.915	57.456	1.00 76.19	H
ATOM	1805	CD	GLU	23	125.807	26.370	58.853	1.00 92.47	H
MOTA	1806	OE1	GLU	23	124.810	26.025	59.525	1.00 98.93	H
ATOM	1807	OE2	GLU	23	126.982	26.286	59.278	1.00.99.99	H
ATOM	1808	C	GLU	23	123.723	29.675	57.962	1.00 47.05	H
MOTA	1809	0	GLU	23	124.610	29.940	58.777	1.00 50.01	H
ATOM	1810	N	ALA	24	122.472	30.117	58.060	1.00 39.44	H
ATOM	1811	CA	ALA	24	122.022	30.980	59.143	1.00 43.91	H
ATOM	1812	CB	ALA	24	120.770	31.729	58.709	1.00 40.39	H
ATOM	1813	C	ALA	24	121.745	30.197	60.429	1.00 49.01	H
ATOM	1814	0	ALA	24	121.532	28.983	60.398	1.00 44.02	H
ATOM	1815	N	SER	25	121.752	30.909	61.555	1.00 60.65	H
ATOM	1816	CA	SER	25	121.504	30.321	62.872	1.00 64.10	H
ATOM	1817	CB .	SER	25	122.557	29.250	63.192	1.00 76.12	H
ATOM	1818	OG	SER	25 ,	123.782	29.512	62.529	1.00 87.44	H
MOTA	1819	C	SER	25	121.514	31.391	63.966	1.00 53.28	H
ATOM	1820	0	SER	25	122.520	32.068	64.188	1.00 50.41	H
ATOM	1821	N	GLY	26	120.384	31.533	64.651	1.00 46.94	H
ATOM	1822	CA	GLY .	26	120.275	32.520	65.708	1.00 30.92	H
MOTA	1823	C	GLY	26	119.044	33.377	65.502	1.00 32.69	H
MOTA	1824	0	GLY	26	118.711	34.201	66.349	1.00 19.54	H
ATOM	1825	N	TYR	27	118.372	33.167	64.370	1.00 42.28	H
MOTA	1826	CA	TYR	27	117.163	33.909	64.012	1.00 45.58	. H
ATOM	1827	CB-	TYR	27	117.546	35.240	63.346	1.00 51.85	H
MOTA	1828	CG :	TYR	27	118.025	35.116	61.907	1.00 59.01	H
ATOM	1829	CD1	TYR	27	117.155	35.345	60.838	1.00 52.27	H
MOTA	1830	CE1	TYR	27	117.595	35.261	59.514	1.00 42.40	H
MOTA	1831	CD2	TYR	27	119.355	34.794	61.614	1.00 52.66	. H
MOTA .	1832 .	CE2	TYR	27	119.804	34.710	60.293	1.00 46.26	H
ATOM	1833	CZ	TYR	27	118.919	34.947	59.250	1.00 50.61	H
MOTA	1834	OH	TYR -	27	119.363	34.893	57.947	1.00 42.85	H
MOTA	1835	C	TYR	27	116.250	33.109	63.072	1.00 48.20	H
ATOM	1836	O	TYR	27	116.553	31.963	62.712	1.00 30.85	H
MOTA	1837	N	THR	28	115.131	33.722	62.684	1.00 47.35	H
ATOM	1838	CA	THR	28	114.176	33.088	61.776	1.00 41.83	H
ATOM	1839	CB	THR	28	112.786	33.737	61.871	1.00 39.96	H
MOTA	1840	OG1	THR	28	112.270	33.577	63.197	1.00 50.93	H
MOTA	1841	CG2	THR	28	111.830	33.084	60.878	1.00 45.16	H
MOTA	1842	C	THR	28	114.653	33.204	60.328	1.00 40.89	H
MOTA	1843	0	THR	28	114.619	34.280	59.739	1.00 31.24	H
MOTA	1844	N	PHE	29	115.095	32.084	59.766	1.00 41.61	H
MOTA	1845	CA	PHE	29	115.591	32.035	58.399	1.00 41.45	H
MOTA	1846	CB	PHE	29	115.946	30.593	58.034	1.00 30.51	H
MOTA	1847	CG	PHE	29	116.611	30.449	56.696	1.00 37.17	H
MOTA	1848	CD1	PHE	29	117.833	31.065	56.439	1.00 30.37	H

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MOTA	1849	CD2	PHE	• ,	29		116.032	29.667	55.700	1.00	36.28	•	H
MOTA	1850	CE1	PHE	ż	29		118.469	30.904	55.214	1.00	21.32		H
MOTA	1851	CE2	PHE		29.	ż	116.666	29.500	54.463	1.00	41.18		H
MOTA	1852	CZ	PHE		29		117.889	30.122	54.225	1.00	35.05		H
MOTA	1853	C	PHE		29		114.594	32.572	57.379	1.00	54.24		H
ATOM	1854	0	PHE		29		114.952	33.331	56.480	1.00	66.70		H
MOTA	1855	N	THR		30		113.342	32.164	57.527	1.00	55.99		H
MOTA	1856	CA	THR		30	•	112.276	32.557	56.615	1.00	52.36		H
MOTA	1857	CB	THR		30		111.052	31.652	56.824	1.00	53.76		H
MOTA	1858	OG1	THR		30		110.733	31.583	58.225	1.00	35.56		H
MOTA	1859	CG2	THR		30		111.357	30.244	56.304	1.00	44.72		H
MOTA	1860	C	THR		30		111.829	34.016	56.703	1.00	47.50		H
MOTA	1861	0	THR		30		110.914	34.426	55.996	1.00	53.11		H
ATOM	1862	N	SER		31		112.470	34.804	57.554	1.00	46.37		H
MOTA	1863	CA	SER		31		112.094	36.207	57.697	1.00	45.74	•	H
ATOM	1864	CB	SER		31		111.832	36.521	59.167	1.00	29.27		H
ATOM	1865	OG	SER		31		110.583	37.159	59.337	1.00	47.69		H
MOTA	1866	C	SER		31		113.143	37.175	57.150	1.00	47.78		H
ATOM	1867	0	SER		31		113.149	38:358	57.509	1.00	46.57		H
MOTA	1868	N	TYR		32		114.027	36.683	56.286	1.00	31.83		H
ATOM	1869	CA	TYR	.0	32		115.068	37.530	55.720	1.00	30.55		H H
MOTA	1870	CB	TYR		32		116.287	37.556	56.642	1.00	32.62 37.51		H
ATOM	1871	CG	TYR		32	£	116.075	38.248	57.963 59.031	1.00	33.89		H
ATOM	1872	CD1	TYR		32		115.494	37.579	60.266	1.00	35.72		H
ATOM	1873	CE1	TYR		32		115.358	38.184	58.166	1.00	39.03		H
ATOM	1874	CD2	TYR		32		116.510	39.556 40.173	59.401	1.00	40.85		H
ATOM	1875	CE2	TYR		32		116.378 115.803	39.476	60.449	1.00	43.40		H
MOTA	1876	CZ	TYR		32		115.603	40.053	61.695	1.00	55.17		H
MOTA	1877	OH	TYR		32 32		115.526	37.071	54.342	1.00	42.11	•	H
ATOM	1878	C .	TYR TYR	4	32	•	115.438	35.889	54.012	1.00	37.33		H
ATOM ATOM	1879 1880	N	TYR		33		116.021	38.017	53.545	1.00	52.12		H
ATOM	1881	CA	TYR	•	33		116.544	37.721	52.210	1.00	50.02		H
ATOM	1882	CB	TYR		33		116.576	38.960	51.309	1.00	42.85		H
ATOM	1883	CG	TYR		33		115.263	39.601	50.944	1.00	58.80		H
ATOM	1884	CD1	TYR		33	1 2	114.637	39.313	49.730	1.00	66.77		H
ATOM	1885	CE1	TYR	•	33		113.466	39.968	49.345	1.00	69.61		H
ATOM	1886	CD2	TYR		33		114.683	40.558	51.771	1.00	76.77		H
ATOM	1887	CE2	TYR	•	33	4	113.513	41.220	51.398		80.20		H
ATOM	1888.	CZ	TYR		33		112.909	40.921	50.185	1.00	74.03		H
ATOM	1889	OH	TYR		33		111.746	41.574	49.830	1.00	56.44	v	H
ATOM	1890	C	TYR	1 **	33		118.000	37.359	52.441	1.00	53.48	•	H
ATOM	1891	0	TYR		33		118.601	37.825	53.411	1.00	55.64		H
ATOM	1892	N	ILE		34		118.574	36.538	51.570	1.00	39.36		H
MOTA	1893	CA	ILE		34		119.991	36.237	51.705	1.00	36.92		H
MOTA	1894	CB	ILE		34		120.310	34.720	51.687	1.00	41.72		H
MOTA	1895	CG2	ILE	v	34		121.831	34.515	51.776	1.00	24.87		H
ATOM	1896	CG1	ILE		34		119.647	34.023	52.879	1.00	33.33		H
MOTA	1897	CD1	ILE		34		120.435	34.137	54.177	1.00	29.68		H
ATOM	1898	C	ILE		34		120.629	36.900	50.490	1.00	33.61		H
MOTA	1899	0	ILE		34		120.304	36.568	49.351	1.00	36.71		H
ATOM	1900	N	HIS		35		121.506	37.864	50.739	1.00	34.93		H
ATOM	1901	CA	HIS		35		122.185	38.573	49.666	1.00	29.41		H
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MOTA	1902	CB	HIS	35	Ì	122.300	40.062	49.990	1.00	22.47	H
MOTA	1903	CG	HIS	35	•	120.983	40.768	50.047	1.00	28.34	H
ATOM	1904	CD2	HIS	35		120.082	40.885	51.049	1.00	17.42	H
ATOM	1905	ND1	HIS	35		120.446	41.427	48.965	1.00	34.24	H
ATOM	1906	CE1	HIS	35		119.266	41.924	49.298	1.00	35.85	H
ATOM ·	1907	NE2	HIS	35		119.023	41.609	50.556	1.00	28.90	H
ATOM	1908	C	HIS	35		123.574	38.000	49.482	1.00	24.58	H
MOTA	1909	O ,	HIS	35		124.156	37.437	50.403	1.00	40.74	H
MOTA	1910	N	TRP	36		124.104	38.149	48.282	1.00	18.85	H
ATOM	1911	CA	TRP	36		125.430	37.664	47.984	1.00	25.49	H
MOTA	1912	CB	TRP	36		125.334	36.410	47.104	1.00	38.00	H
ATOM	1913	CG	TRP	36		125.226	35.122	47.882	1.00	42.56	H
ATOM	1914	CD2	TRP	36		126.288	34.433	48.564	1.00	28.82	H
ATOM	1915	CE2	TRP	36		125.730	33.274	49.146	1.00	18.67	H
ATOM	1916	CE3	TRP	36		127.658	34.687	48.737	1.00	34.82	H
ATOM	1917	CD1	TRP	36	ı	124.097	34.368	48.075	1.00	40.81	H
ATOM	1918	NE1	TRP	36		124.394	33.257	48.834	1.00	30.56	H
MOTA	1919	CZ2	TRP	36		126.492	32.368	49.889	1.00	44.00	H
MOTA	1920	CZ3	TRP	36		128.418	33.786	49.479	1.00	41.71	H
MOTA	1921	CH2	TRP	36		127.832	32.641	50.045	1.00	49.64	H
MOTA	1922	C	TRP	3,6		126.189	38.784	47.269	1.00	22.21	H
MOTA	1923	0	TRP	36		125.658	39.410	46.352	1.00	20.33	H
ATOM	1924	N	VAL	37·		127.420	39.044	47.703	1.00	21.22	H
MOTA	1925	CA	VAĻ	37		128.237	40.085	47.089	1.00	29.63	H
MOTA	1926	CB	VAL	37		128.157	41.414	47.887	1.00	30.69	H
MOTA	1927	CG1	VAL	37	ı	126.874	41.453	48.701	1.00	7.82	H
MOTA	1928	CG2	VAL	37		129.366	41.569	48.780	1.00		H
MOTA	1929	C	VAL	37		129.693	39.641	46.984		33.49	H
MOTA	1930	.0	VAL	37		130.223	39.017	47.900	1.00	17.14	H
MOTA	1931	N	LYS	38	-	130.330	39.970	45.862	1.00	43.70	H
MOTA	1932	CA	LYS	38	*	131.720	39.591	45.619	1.00		H
MOTA	1933	CB	LYS	38		131.849	38.932	44.233	1.00		H
MOTA	1934	CG	LYS	38		132.592	39.756	43.175	1.00		H
ATOM	1935	CD	LYS	38		133.109	38.890	42.022	1.00		H
MOTA	1936	CE	LYS	38		131.967	38.347	41.155	1.00		H
MOTA	1937	NZ	LYS	3,8		132.372	37.162	40.335	1.00		H
MOTA	1938	C	LYS	38		132.699	40.757	45.732	1.00		H
ATOM	1939	, O	LYS	38		132.467	41.837	45.189	1.00		H
MOTA	1940	N	GLN	39		133.798	40.525	46.439		38.36	H
MOTA	1941	CA	GLN	39		134.819		46.621		30.47	H
MOTA	1942	CB	GLN	39		134.969	41.879			40.49	H
MOTA	1943	CG	GLN	39		136.078	42.863	48.409		23.44	H
MOTA	1944	CD	GLN	39		135.965	43.424	49.803		27.61	H
ATOM	1945	OE1	GLN	39		135.386	44.485	50.004		26.42	H
MOTA	1946	NE2	GLN	39		136.517	42.709	50.781		31.89	H
ATOM	1947	C	GLN	39		136.142	41.029	46.074		29.22	H
MOTA	1948	0	GLN	39		136.781	40.160	46.672		19.00	H
MOTA	1949	N	ARG	40		136.548	41.560	44.928		41.18	H
MOTA	1950	CA	ARG	40		137.794	41.139	44.310		48.75	H
MOTA	1951	CB	ARG	40		137.805	41.496	42.819	1.00		H
MOTA	1952	CG	ARG	40		137.203	40.422	41.923	1.00		H
MOTA	1953	CD	ARG	40	ı	137.409	40.741	40.448	1.00		H
MOTA	1954	NE	ARG	40		138.762	40.415	39.997	1.00	66.96	H

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ATOM	1955	CZ	ARG	40	139.215	39.178	39.816	1.00	59.13	H
ATOM	1956	NH1	ARG	40	138.426	38.137	40.046	1.00	49.49	H
ATOM	1957	NH2	ARG	40	140.459	38.982	39.400	1.00	64.52	H
ATOM	1958	C	ARG	40	138.971	41.791	45.024	1.00	49.05	·H
ATOM	1959	.0	ARG	40	138.955	42.989	45.312	1.00	41.67	H
ATOM	1960	N.	PRO	41	140.007	40.996	45.329	1.00	49.95	H
MOTA	1961	CD	PRO	41	140.102	39.557	45.022	1.00	60.26	H
ATOM	1962	CA	PRO	41	141.200	41.485	46.013	1.00	40.75	H
ATOM	1963	CB	PRO	41	142.268	40.476	45.625	1.00	50.53	H
ATOM	1964	CG	PRO	41	141.516	39.202	45.415	1.00	62.82	H
ATOM	1965	C	PRO	41	141.558	42.888	45.576	1.00	38.02	H
ATOM	1966	0	PRO	41	141.769	43.147	44.392	1.00	47.09	H
	1967	И	GLY	42	141.614	43.794	46.542	1.00	36.72	H
ATOM	1968	CA	GLY	42	141.952	45.170	46.241	1.00	31.35	H
ATOM	1969	CA	GLY	42	140.726	45.981	45.900	1.00	40.05	Н
ATOM			GLY	42	140.468	47.014	46.514	1.00	41.40	H
ATOM	1970	O,	GLN	43	139.975	45.502	44.913	1.00	58.75	Н
ATOM	1971	N		43	138.752	46.163	44.468	1.00	67.06	Н
ATOM	1972	CA	GLN	43	138.192	45.449	43.227	1.00	64.21	H
ATOM	1973	CB	GLN		137.035	46.178	42.540	1.00	71.56	H
'ATOM	1974	CG	GLN	43	137.033	45.251	42.130	1.00	71.51	H
MOTA	1975	CD	GLN	43	135.330	44.540	42.963	1.00	67.00	H
ATOM	1976	OE1	GLN	43	135.566	45.255	40.842	1.00	53.00	H
ATOM	1977	NE2	GLN	43 ,	137.701	46.158	45.581	1.00	68.90	H
ATOM	1978	C	GLN	43	137.782	45.366	46.521	1.00	72.87	H
ATOM	1979	Q NT	GLN	43	137.782	47.055	45.471	1.00	67.47	H
MOTA	1980	N	GLY	44		47.033	46.458	1.00	54.03	H
ATOM	1981	CA	GLY	44	135.661		46.268	1.00	52.55	H
ATOM	1982	C	GLY	44	134.746	45.927	45.794	1.00	65.13	H
ATOM	1983	0	GLY	. 44	135.191	44.881	46.623	1.00		H
ATOM	1984	N	LEU	45	133.474	46.062	46.456	1.00	50.12	H
MOTA	1985	CA	LEU	45	132.552	44.946 44.339	47.819	1.00	44.25	H
ATOM	1986	CB	LEU	45	132.197		48.790	1.00	36.87	H
MOTA	1987	CG	LEU	45	131.306	45.109	50.212	1.00	34.38	H
ATOM	1988	CD1	LEU	45	131.661	44.692	48.597	1.00	31.30	H
MOTA	1989	CD2	LEU	45	131.480	46.605	45.689	1.00	47.35	H
ATOM	1990	G .	LEU	45	131.283	45.315	45.656	1.00	52.97	H
MOTA	1991	0	LEU	45	130.876	46.475		1.00	38.18	H
MOTA	1992	N	GLU	46	130.673	44.311	45.066			H
MOTA	1993	CA	GLU	46	129.468	44.497	44.275	1.00		· H
MOTA	1994	CB	GLU	46	129.779	44.312	42.787	1.00		H
MOTA	1995	CG -	GLU	46	131.106	43.601	42.502	1.00	70.14	H
MOTA	1996	CD	GLU	46	131.544	43.722	41.050	1.00		H
MOTA	1997	OE1		46	132.769	43.760	40.796	1.00		Н
MOTA	1998	OE2		46	130.660	43.778	40.171	1.00		H
MOTA	1999	C	GLU	46	128.400	43.506	44.686	1.00		
MOTA	2000	0	GLU	. 46	128.697	42.477	45.293	1.00		H
MOTA	2001	N	TRP	47	127.157	43.818	44.329	1.00		H
MOTA	2002	CA	TRP	47	126.010	42.982	44.661	1.00		H
MOTA	2003	CB	TRP	47	124.794	•	44.906	1.00		H
MOTA	2004	CG	TRP	47	123.538	43.163	45.304	1.00		H
MOTA	2005	CD2	TRP	47	122.417	42.881	44.459		46.71	H
ATOM	2006	CE2	TRP	47	121.440	42.259	45.262		40.21	H
MOTA	2007	CE3	TRP	47	122.148	43.096	43.104	1.00	44.16	H

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ATOM	2008	CD1	TRP	47	123.204	42.709	46.547	1.00 44.85	H
MOTA	2009	NEl	TRP	47	121.942	42.165	46.533	1.00 44.22	H
MOTA	2010	CZ2	TRP	47	120.205	41.852	44.750	1.00 48.68	H
MOTA	2011	CZ3	TRP	47	120.924	42.689	42.597	1.00 48.92	H
MOTA	2012	CH2	TRP	47	119.969	42.073	43.420	1.00 39.77	H
MOTA	2013	C	TRP	47	125.692	41.936	43.592	1.00 45.09	H
MOTA	2014	Ο,	TRP	47	125.359	42.260	42.449	1.00, 45.19	H
MOTA	2015	N	ILE	48	125.800	40.671	43.981	1.00 45.61	H
ATOM	2016	CA	ILE	48	125.529	39.562	43.080	1.00 37.68	H
ATOM	2017	CB	ILE	48	126.185	38.266	43.601	1.00 25.87	H
MOTA	2018	CG2	ILE	48	125.479	37.039	43.036	1.00 23.09	H
MOTA	2019	CG1	ILE	48	127.657	38.249	43.202	1.00 15.27	H
MOTA	2020	CD1	ILE	48	128.449	37.133	43.847	1.00 20.12	H
ATOM	2021	C	ILE	48	124.028	39.356	42.936	1.00 35.05	H
ATOM	2022	0	ILE	48	123.461	39.591	41.870	1.00 41.96	H
MOTA	2023	N	GLY	49	123.388	38.918	44.013	1.00 32.61	H
MOTA	2024	CA	GLY	49	121.953	38.689	43.986	1.00 30.75	H
MOTA	2025	C	GLY	49	121.432	38.298	45.359	1.00 38.37	H
ATOM	2026	0	GLY	49	122.161	38.327	46.349	1.00 41.94	H
MOTA	2027	N	CYS	50	120.163	37.931	45.431	1.00 37.54	H
MOTA	2028	CA	CYS	50	119.587	37.540	46.705	1.00 38.40	H
ATOM	2029	CB	CYS	50	119.095	38.774	47.462	1.00 51.77	H
ATOM	2030	SG	CYS	50	117.500	39.407	46.877	1.00 50.59	H
ATOM	2031	C	CYS	50	118.438	36.577	46.500	1.00 42.42	H
ATOM	2032	0	CYS	50	117.835	36.535	45.431	1.00 50.09	H
MOTA	2033	N	ILE	. 51	118.146	35.804	47.537	1.00 42.92	H
MOTA	2034	CA	ILE	51	117.059	34.837	47.502	1.00 37.44	H
ATOM	2035	CB	ILE	51	117.596	33.380	47.377	1.00 28.69	H
ATOM	2036	CG2	ILE	51	118.648	33.111	48.440	1.00 29.15	H
ATOM	2037	CG1	ILE	51	116.448	32.382	47.521	1.00 22.13	H
ATOM	2038	CD1	ILE	51	115.840	31.963	46.201	1.00 43.28	H
ATOM	2039	C	ILE	51	116.277	34.989	48.800	1.00 42.00	H
ATOM	2040	0	ILE	51	116.861	35.219	49.868	1.00 34.19	H
ATOM	2041	N	TYR	52	114.957	34.886	48.706	1.00 38.73	H
ATOM	2042	CA	TYR	52	114.124	35.013	49.888	1.00 34.95	H
MOTA	2043	CB	TYR	52	112.954	35.960	49.643	1.00 26.98	H
ATOM	2044	CG	TYR	. 52	112.041	36.049	50.840 52.132	1.00 28.39 1.00 31.39	H H
ATOM	2045 2046	CD1 CE1	TYR TYR	52 52	112.571 111.752	36.155 36.193	53.244	1.00 31.39	H
ATOM			TYR	, 52	110.660	35.986	50.695	1.00 43.44	'. H
ATOM .	2047	CD2		52	109.821	36.022	51.800	1.00 43.98	H
ATOM	2048 2049	CE2	TYR TYR	52 52	110.376	36.124	53.075	1.00 45.98	H
ATOM	2049	CZ OH	TYR	52 52	109.556	36.153	54.178	1.00 50.97	H
ATOM	r			52 52	113.578	33.674	50.350	1.00 37.54	H
MOTA	2051	С О	TYR	52 52	112.611	33.161	49.791	1.00 45.44	H
ATOM	2052		TYR		114.191	33.101	51.386	1.00 46.32	H
ATOM	2053	N	PRO	53 . = 2		33.610	52.137	1.00 48.32	H
ATOM	2054	CD	PRO	53 53	115.347		51.900		H
ATOM ATOM	2055 2056	CA CB	PRO PRO	53 53	113.728 114.599	31.803 31.566	53.126	1.00 36.81 1.00 38.59	H
ATOM	2056	CG	PRO	53 ·	115.817	32.404	52.894	1.00 59.97	H
ATOM	2057	C	PRO	53 53	112.279	31.971	52.275	1.00 35.25	H
ATOM	2059	0	PRO	53	111.926	32.927	52.959	1.00 33.23	H
ATOM	2059	N	GLY	54	111.441	31.055	51.815	1.00 37.30	H
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	ATOM	2061	CA	GLY	¹ . 54	110.027	31.142	52.120	1.00 53.47	ŢΉ	•
	ATOM	2062	C	GLY	54	109.200	31.023	50.860	1.00 58.70	H	
d T	ATOM	2063	0	GLY	54	108.726	29.936	50.530	1.00 74.82	H	
	ATOM	2064	\mathbf{N}_{\cdot}	ASN	55	109.021	32.132	50.150	1.00 48.62	H	
٠	ATOM	2065	CA	ASN	55	108.248	32.116	48.917	1.00 45.89	H	•
	ATOM	2066	CB	ASN	55	107.602	33.482	48.675	1.00 46.66	H	
	ATOM	2067	CG	ASN	55	108.344	34.312	47.658	1.00 46.59	H	
	ATOM	2068	OD1	ASN	55	109.183	35.138	48.009	1.00 50.93	H	
~	ATOM	2069	ND2	ASN	55	108.027	34.107	46.384	1.00 65.32	H	
	ATOM	2070.	C	ASN	55	109.177	31.740	47.777	1.00 59.93	H	
	ATOM	2071	0	ASN	55	108.738	31.536	46.645	1.00 70.19	H	
	ATOM	2072	N	VAL	56	110.466	31.644	48.110	1.00 68.48	H	
	ATOM	2073	CA	VAL	56	111.541	31.269	47.182	1.00 68.32	H	
	ATOM	2074	CB	VAL	56	111.181	29.960	46.416	1.00 73.69	H	
	ATOM	2075	CG1		56	110.739	30.271	44.989	1.00 75.39	H	
	ATOM	2076	CG2		56	112.377	29.021	46.415	1.00 57.36	H	
	ATOM	2077	C	VAL	56	111.958	32.352	46.182	1.00 64.26	H	
	ATOM	2078	0	VAL	56	112.859	32.142	45.366	1.00 50.69	H	
	ATOM	2079	N	ASN	57	111.307	33.511	46.258	1.00 70.60	H	
	ATOM	2080		ASN	57	111.610	34.622	45.366	1.00 62.78	H	
	ATOM	2081	CB.	ASN	57	110.996	35.913	45.898	1.00 76.22	\cdot H $^{\circ}$	·
r	ATOM	2082	CG	ASN	57	109.868	36.422	45.032	1.00 82.20	H	
	ATOM	2083		ASN	57	109.018	37.191	45.486	1.00 72.33	H	
**	ATOM	2084		ASN	57	109.849	35.989	43.772	1.00 72.74	H .	
*	ATOM	2085	C	ASN	57	113.110	34.795	45.242	1.00 63.32	H	1
	ATOM	2086	0.	ASN	57	113.857	34.515	46.181	1.00 68.16	H	
	ATOM	2087	N	THR	58	113.553	35.267	44.084	1.00 54.53	Н	
	ATOM	2088	CA	THR	58	114.974	35.465	43.859	1.00 52.32	H	
**	ATOM	2089	CB	THR	58	115.597	34.191	43.279	1.00 48.24	H	
	ATOM	2090	OG1	THR	58	116.806	34.523	42.594	1.00 45.77	H	
÷	ATOM	2091	CG2	THR	58 ·	114.628	33.516	42.314	1.00 53.99	H	•
	ATOM	2092	C	THR	58	115.243	36.641	42.921	1.00 52.31	H	•
•	ATOM	2093	0	THR	58	114.436	36.935	42.039	1.00 59.83	H	ý
	ATOM	2094	N	ASN	59	116.375	37.313	43.117	1.00 40.59	H	e de la companya de l
۵	ATOM	2095	CA	ASN	59	116.730	38.462	42.290	1.00 38.18	H	\$
	ATOM	2096	CB	ASN	5 <i>9</i>	116.330	39.758	42.998	1.00 53.76	H H	·
		2090	i	ASN	59	114.928	40.217	42.632	1.00 53.44	H	
e .	ATOM	2097	OD1		5 <i>9</i>	114.712	40.809	41.572	1.00 58.59	H	
۶	MOTA	•		ASN	5 <i>9</i>	113.970	39.951	43.512	1.00 44.63	H	
	ATOM	2099			5 <i>9</i>	118.217	38.505	41.970	1.00 30.27	H	
	ATOM	2100	C	ASN	'	119.049	38.423	42.873	1.00 35.55	H	
	ATOM	2101	O	ASN	<i></i>	118.544	38.661	40.687	1.00 19.72	H -	ı
	ATOM	2102	N	TYR	60	119.935	38.710	40.243	1.00 19.72	H	ı
	ATOM	2103	CA	TYR	60 ,	120.213	37.596	39.227	1.00 27.47	H	
•	ATOM	2104	CB	TYR	60 60		36.215	39.675	1.00 27.47	H	
	ATOM	2105	CG	TYR	60	119.809		39.929	1.00 18.79	H	•
	ATOM	2106		TYR	60	120.762	35.233	40.325	1.00 40.31	H	
	ATOM	2107		TYR	60	120.382	33.951		1.00 40.64	H	ą
	ATOM	2108	CD2		60	118.468	35.883	39.825		H	1
	ATOM	2109	CE2	TYR	60	118.077	34.611	40.217	1.00 47.25	H H	
	ATOM	2110	CZ	TYR	60	119.033	33.647	40.469	1.00 51.22		-
•	ATOM	2111	OH	TYR	60	118.621	32.391	40.883	1.00 56.18	H	
	ATOM	2112	C	TYR	60	120.367	40.034	39.618	1.00 25.63	H	
ч	ATOM	2113	0	TYR	60	119.574	40.746	39.008	1.00 17.78	H	
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MOTA	2114	\mathbf{N}_{\downarrow}	ASN	61	121.645	40.354	39.789	1.00 31.77	H
ATOM	2115	CA	ASN	61	122.224	41.551	39.213	1.00 30.42	H
MOTA	2116	CB	ASN	61	123.542	41.891	39.907	1.00 26.96	H
ATOM	2117	CG	ASN	61	124.176	43.155	39.367	1,00 28.98	H
MOTA	2118	OD1	ASN	61	124.721	43.964	40.120	1.00 39.03	H
MOTA	2119	ND2	ASN	61	124.105	43.335	3,8.052	1.00 39.88	H
MOTA	2120	C	ASN	61	122.480	41.102	37.787	1.00 42.86	H
MOTA	2121	0 .	ASN	61	123.062	40.041	37.571	1.00 56.00	H
MOTA	2122	N	GLU	62	122.045	41.889	36.812	1.00 46.51	H
ATOM	2123	CA	GLU _,	62	122.224	41.498	35.424	1.00 52.07	H
MOTA	2124	CB	GLU	62	121.511	42.490	34.504	1.00 57.39	H
ATOM	2125	CG	GLU	62	120.513	41.839	33.531	1.00 76.62	H
ATOM	2126	CD	GLU	62	119.280	41.242	34.214	1.00 81.14	H
ATOM	2127	OE1	GLU	62	119.442	40.484	35.197	1.00 79.43	H
ATOM	2128	OE2	GLU	62	118.148	41.528	33.759	1.00 70.90	H
ATOM	2129	C	GLU	62	123.678	41.327	35.000	1.00 53.65	H
MOTA	2130	0	GLU	62	123.953	40.991	33.847	1.00 75.05	H
ATOM	2131	N	LYS	63	124.610	41.543	35.922	1.00 36.05	H
ATOM	2132	CA	LYS	63	126.025	41.379	35.604	1.00 35.02	H
ATOM	2133	CB	LYS	63	126.862	42.421	36.353	1.00 26.34	H
ATOM	2134	CG	LYS	63	127.215	43.653	35.532	1.00 49.15	H
ATOM	2135	CD	LYS	63	126.773	44.948	36.217	1.00 45.62	H
ATOM	2136	CE .	LYS	63	127.938	45.619	36.920	1.00 40.94	H
MOTA	2137	NZ	LYS	63	128.652	44.625	37.772	1.00 39.59	H
ATOM	2138	C	LYS	63	126.506	39.969	35.961	1.00 40.58	H
ATOM	2139	0	LYS	63	127.618	39.576	35.611	1.00 45.93	H H
ATOM	2140	N	PHE	64	125.657	39.214	36.658	1.00 47.98	H
ATOM	2141	CA	PHE	64	125.975	37.849 37.789	37.073 38.579	1.00 42.86 1.00 42.85	H
MOTA	2142	CB	PHE	64	126.263 127.177	38.872	39.068	1.00 42.85	H
MOTA	2143	CG	PHE	64 64	128.538	38.831	38.791	1.00 50.59	H
ATOM	2144 2145	CD1 CD2	PHE PHE	64	126.536	39.929	39.817	1.00 38.08	H
ATOM ATOM	2145	CE1	PHE	64	129.388	39.830	39.255	1.00 35.00	H
ATOM	2147	CE2	PHE	64	127.524	40.933	40.284	1.00 43.09	H
ATOM	2147	CEZ	PHE	.64	128.877	40.883	40.004	1.00 43.03	H
ATOM	2149	G.	PHE	64	124.823	36.908	36.768	1.00 43.11	H
ATOM	2149	0	PHE	64	124.560	35.988	37.535	1.00 47.33	H
ATOM	2151	N	LYS	65 [°]	124.148	37.128	35.644	1.00 55.21	H
ATOM	2152	CA	LYS	65	123.005	36.302	35.259	1.00 59.07	H
ATOM	2153	CB	LYS	65	122.383	36.806	33.949	1.00 45.97	H
ATOM	2154	CG	LYS	65	123.146	37.914	33.251	1.00 49.55	H
ATOM	2155	CD	LYS	65	124.165	37.363	32.270	1.00 46.70	H
MOTA	2156	CE	LYS	65	125.116	38.461	31.811	1.00 50.30	H
MOTA	2157	NZ	LYS	65	125.548	38.271	30.398	1.00 58.93	H
ATOM	2158	C	LYS	65	123.279	34.802	35.118	1.00 67.16	H
MOTA	2159	0	LYS	65	122.598		35.741	1.00 70.12	H
ATOM	2160	N	ASP	66	124.267	34.440	34.304	1.00 69.41	H
MOTA	2161	CA	ASP	66	124.579	33.031	34.073	1.00 66.83	H
ATOM	2162	CB	ASP	66	125.508	32.898	3.2.872	1.00 66.07	Н
MOTA	2163	CG	ASP	66	124.747	32.712	31.580	1.00 66.45	· H
ATOM	2164	OD1	ASP	66	124.869	31.628	30.973	1.00 66.35	H
ATOM	2165	OD2	ASP	66	124.023	33.649	31.177	1.00 50.12	Н
ATOM	2166	C	ASP	66	125.168	32.265	35.251	1.00 70.25	H

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MOTA	2167	0	ASP	66 🐫 .	124.514	31.365	35.792	1.00	72.29	· H
ATOM	2168	N	LYS	67	126.399	32.605	35.637	1.00	62.38	H
ATOM	2169	CA	LYS	67	127.071	31.934	36.750	1.00	49.02	H
ATOM	2170	CB	LYS	67	128.374	32.653	37.115	1.00	25.39	H
ATOM	2171	CG	LYS	67	128.541	34.034	36.489	1.00	48.63	H
ATOM	2172	CD	LYS	67	129.958	34.579	36.675	1.00	21.16	H
ATOM	2173	CE	LYS	67	130.912	34.018	35.624	1.00	43.17	H
ATOM	2174	NZ	LYS	67	132.251	33.618	36.179	1.00	34.20	H
ATOM	2175	C	LYS	67	126.178	31.887	37.977	1.00	59.48	H
ATOM	2176	0	LYS	67	125.721	30.816	38.390	1.00	51.12	H
MOTA	2177	N	ALA	68	125.929	33.066	38.545	1.00	67.14	H
ATOM	2178	CA	ALA -	68	125.104	33.220	39.741	1.00	54.74	H
MOTA	2179	CB	ALA	68	125.017	34.688	40.108	1.00	54.84	H
ATOM	2180	C	ALA	68	123.701	32.631	39.631	1.00	49.40	H
MOTA	2181	0	ALA	68	122.851	33.136	38.896	1.00	58.08	H
ATOM	2182	N	THR	69	123.473	31.564	40.387	1.00	32.05	H
MOTA	2183	CA	THR	69	122.192	30.874	40.429	1.00	37.56	H
MOTA	2184	CB	THR	69	122.284	29.541	39.655	1.00	35.94	H
MOTA	2185	OG1	THR	69	122.392	29.821	38.253	1.00	40.10	H
MOTA	2186	CG2	THR	69	121.065	28.676	39.908	1.00	26.92	H
MOTA	2187	C	THR	69	121.915	30.626	41.914	1.00	43.54	H
MOTA	2188	0	THR	69	122.595	29.823	42.550	1.00	40.52	H
ATOM	2189	N	LEU	70	120.924	31.319	42.469	1.00	45.97	H
ATOM	2190	CA	LEU	70	120.622	31.189	43.893	1.00	46.62	H
MOTA	2191	CB	LEU	70	120.166	32.536	44.445	1.00	47.28	H
MOTA	2192	CG	LEU	70	121.305	33.331	45.091	1.00	55.81	H
MOTA	2193	CD1	LEU	70	121.133	34.805	44.767	1.00	43.73	H
MOTA	2194	CD2	LEU	70	121.322	33.094	46.611	1.00	43.94	H
ATOM	2195	C	LEU	70	119.636	30.107	44.312	1.00	43.94	H
MOTA	2196	0	LEU	70	118.496	30.070	43.849	1.00	42.32	H
MOTA	2197	N	ILE	71	120.103	29.247	45.218	1.00	44.21	H
MOTA	2198	CA	ILE	71	119.333	28.125	45.755	1.00	49.89	H
MOTA	2199	CB	ILE	71 .	120.026	26.770	45.430	1.00	51.60	H
MOTA	2200	CG2	ILE	71	119.259	25.616	46.072	1.00	29.06	H
MOTA	2201	CG1	ILE	71	120.107	26.573	43.911	1.00	54.43	H
ATOM	2202	CD1	ILE	71	121.184	27.402	43.222	1.00	43.28	H
MOTA	2203	C	ILE	71	119.203	28.255	47.278	1.00	52.79	H
ATOM	2204	0	ILE	71	120.103	28.779	47.939	1.00	62.18	. · H
MOTA	2205	M	VAL	72	118.093	27.768	47.830	1.00	50.92	H
MOTA	2206	CA	VAL	72	117.837	27.843	49.269	1.00	52.77	H
MOTA	2207	CB	VAL	72	116.551	28.677	49.549	1.00	47.96	H
MOTA	2208	CG1	VAL	72	115.313	27.828	49.317	1.00	44.08	·H
MOTA	2209	CG2	VAL	72	116.569	29.224	50.967		43.63	H
ATOM	2210	C	VAL	72	117.687	26.437	49.861	1.00	56.26	H
MOTA	2211	0	VAL	72	117.627	25.457	49.123	1.00	65.48	H
MOTA	2212	N	ASP	73	117.638	26.344	51.191	1.00	56.09	\mathbf{H}
MOTA	2213	CA	ASP	7,3	117.492	25.064	51.891	1.00	50.35	H
MOTA	2214	CB	ASP	73	118.848	24.365	51.995	1.00	53.65	H
MOTA	2215	CG	ASP	73	118.721	22.907	52.384	1.00	57.99	H.
MOTA	2216	OD1	ASP	73	118.119	22.616	53.443	1.00	57.92	H
MOTA	2217	QD2	ASP	73	119.229	22.055	51.625	1.00	61.79	H
ATOM	2218	C .	ASP	73	116.932	25.313	53.290	1.00	50.51	H
ATOM	2219	0	ASP	73	117.664	25.288	54.280	1.00	43.10	H

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MOTA	. 2220 .	N	THR		74		115.624	25.535	53.352	1.00 56.54	H
ATOM	2221	CA	THR		74		114.913	25.836°	54.593	1.00 66.24	H
ATOM	2222	CB	THR		74	3	113.421	26.020	54.296	1.00 71.27	H
ATOM	2223	OG1	THR		74		113.183	25.793	52.901	1.00 71.81	H
ATOM	2224	CG2	THR		74		112.979	27.430	54.659	1.00 81.34	H
ATOM	2225	С	THR		74		115.054	24.876	55.785	1.00 71.66	H
ATOM	2226	O .	THR		74		114.662	25.220	56.902	1.00 67.59	H
ATOM	2227	N	SER		75		115.610	23.689	55.559	1.00 75.40	Ħ
ATOM	2228	CA	SER		75		115.775	22.712	56.634	1.00 69.25	H
ATOM	2229	CB	SER		75		115.833	21.292	56.063	1.00 76.48	H
ATOM	2230	OG	SER		75		116.615	20.445	56.891	1.00 75.33	H
ATOM	2231	C	SER		75		117.024	22.961	57.474	1.00 60.40	H
ATOM	2232	0	SER		75	٠	116.949	23.066	58.703	1.00 51.38	H
MOTA	2233	N	SER		76		118.171	23.040	56.807	1.00 45.77	H
ATOM	2234	CA	SER		76		119.435	23.282	57.498	1.00 44.97	H
ATOM	2235	CB	SER		76		120.585	22.601	56.749	1.00 51.28	H
ATOM	2236	OG	SER		76		120.106	21.807	55.676	1.00 43.07	н
ATOM	2237	C	SER		76		119.691	24.781	57.589	1.00 34.83	H
	2237	0	SER		76		120.755	25.221	58.008	1.00 28.11	H
ATOM			ASN		77		118.697	25.563	57.194	1.00 46.96	
MOTA	2239	N			77		118.826	27.009	57.222	1.00 38.99	
MOTA	2240	CA	ASN		77	,	118.847	27.513	58.665	1.00 41.25	
MOTA	2241	CB	ASN		77		117.459	27.785	59.206	1.00 39.52	H
MOTA	2242	CG	ASN		77	K	116.470	27.733	58.468	1.00 40.29	
ATOM	2243	OD1	ASN				117.377	28.082	60.496	1.00 23.39	
MOTA	2244	ND2	ASN		77		120.111	27.395	56.515	1.00 34.49	
MOTA	2245	C	ASN		77	4	120.111	28.067	57.077	1.00 34.45	:
ATOM	2246	0	ASN	,	77	-		26.944	55.275	1.00 49.07	•
ATOM	2247	N	THR		78		120.240	27.244	54.481	1.00 33.07	
ATOM	2248	CA	THR		78		121.417		54.336	1.00 47.54	
ATOM	2249	CB ·	THR		78		122.340	26.001	53.189	1.00 47.34	
ATOM	2250	OG1	THR		78		121.955	25.239	55.568	1.00 23.72	
ATOM	2251	CG2	THR		78		122.244	25.122		1.00 19.39	
MOTA	`2252	, C .	THR		78		121.030	27.761	53.100		
MOTA	2253	0	THR		78		120.107	27.255	52.465		
MOTA	2254	N	ALA		79		121.738	28.791	52.658	1.00 32.09	
MOTA	2255	CA	ALA		79		121.498	29.399	51.361	1.00 45.71	
MOTA	2256	CB	ALA		79		121.265	30.903	51.520	1.00 20.04	
ATOM	2257	C	ALA		79		122.734	29.148	50.509	1.00 54.97	H
MOTA	2258	0	ALA		79		123.854	29.447	50.927	1.00 71.91	
MOTA	2259	N	TYR		80		122.550	28.589	49.321	1.00 37.02	
ATOM	2260	CA	TYR		80		123.697	28.329	48.480	1.00 32.51	
MOTA	2261	CB	TYR		80		123.635	26.921	47.920	1.00 27.41	
MOTA	2262	CG	TYR		80		123.465	25.846	48.950	1.00 28.36	
MOTA	2263	CD1	TYR		80	,	124.539	25.049	49.332	1.00 30.12	
ATOM	2264	CE1	TYR		80		124.371	24.000	50.232	1.00 47.45	
MOTA	2265	CD2	TYR,		80		122.212	25.575	49.495	1.00 29.76	
MOTA	2266	CE2	TYR	:	80		122.028	24.529	50.394	1.00 40.26	
MOTA	2267	CZ	TYR		80	ı	123.111	23.742	50.759	1.00 45.55	
ATOM	2268	OH	TYR		80		122.933	22.695	51.643	1.00 45.67	-
MOTA	2269	C	TYR		80		123.819	29.307	47.327	1.00 47.49	
MOTA	2270	0	TYR		80		122.870	30.010	46.974	1.00 54.32	
MOTA	2271	N	MET		81		125.012	29.328	46.744	1.00 58.24	
MOTA	2272	CA	MET		81		125.340	30.175	45.609	1.00 51.28	H

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	ATOM	2273	CB	MET	81.	126.117	31.401	46.073	1.00	47.13	H	
	MOTA	2274	CG	MET	81	127.250	31.794	45,151	1.00	49.47	H	1
	ATOM	2275	SD	MET	81 ,	126.890	33.310	44.268	1.00	52.80	H	
	ATOM	2276	CE	MET	,81	127.508	34.508	45.421	1.00	52.92	H	
	ATOM	2277	C ·	MET	81	126.220	29.327	44.699	1.00	51.47	H	
	ATOM	2278	O ,	MET	81	127.342	28.976	45.065	1.00	48.72	H	
	ATOM	2279	N	GLN	82	125.707	28.981	43.525	1.00	46.87	H	
	ATOM	2280	CA	GLN	82	126.476	28.175	42.595	1.00	45.38	H	
	ATOM	2281	CB	GLN	82	125.589	27.113	41.943	1.00	71.53	H	
	ATOM	2282	CG	GLN	82	125.978	26.739	40.511	1.00	89.74	H	
	ATOM	2283	CD	GLN	82	127.278	25.955	40.433	1.00	96.73	H	
	MOTA	2284	OE1	GLN	82	127.925	25.699	41.448	1.00	98.73	H	•
	ATOM	2285	NE2	GLN	82	127.665	25.572	39.220	1.00	94.58	H	
	MOTA	2286	C -	GLN	82	127.075	29.065	41.530	1.00	44.59	H	
	MOTA	2287	0	GLN	82	126.366	29.787	40.833	1.00	42.20	H	
	ATOM	2288	N	LEU	83	128.394	29.014	41.422	1.00	49.17	H	
	ATOM	2289	CA	LEU	83	129.114	29.797	40.434	1.00	46.27	H	
	ATOM	2290	CB	LEU	83	130.369	30.398	41.067	1.00	32.33	H	
	ATOM	2291	CG	LEU	83	130.033	31.416	42.160	1.00	31.17	H	
	ATOM	2292	CD1	LEU	83	131.119	31.455	43.252	1.00	6.90	H	
	ATOM	2293	CD2	LEU	83	129.865	32.766	41.496	1.00	18.19	H	·
	ATOM	2294	C	LEU	83	129.471	28.845	39.298	1.00	45.11	H	
	MOTA	2295	0	LEU	83	130.201	27.870	39.496	1.00	36.84	H	•
	ATOM	2296	N	SER	84	128.925	29.118	38.117	1.00	44.08	H	
	ATOM	2297	CA	SER	84	129.160	28.280	36.948	1.00	46.97	H	
	MOTA	2298	CB	SER	84	127.829	27.869	36.323	1.00	54.37	H	
	ATOM	2299	OG	SER	84	127.604	28.576	35.118	1.00	64.19	H	
	ATOM	2300	С	SER	84	130.037	28.942	35.896	1.00	49.55	\mathbf{H}	
	MOTA	2301	0	SER	84	129.905	30.137	35.617	1.00	47.92	H	,
	ATOM	2302	N	ARG	85	130.925	28.146	35.306	1.00	48.23	H	
	ATOM	2303	CA	ARG	85	131.842	28.637	34.294	1.00	41.86	H	1
	ATOM	2304	CB	ARG	85	131.057	29.141	33.082	1.00	46.21	H	1
	MOTA	2305	CG	ARG	85	130.474	28.012	32.236	1.00	41.59	H	
-	MOTA	2306	CD	ARG	85	129.125	28.393	31.630	1.00	68.47	H	:
	MOTA	2307 .	NE	ARG	85	129.174	28.406	30.170	1.00	68.50	H	
	MOTA	2308	CZ	ARG	85	128.142	28.126	29.381	1.00	60.66	H	
	ATOM	2309	NH1	ARG	85	126.962	27.808	29.906	1.00	56.39	H	
	ATOM	2310	NH2	ARG	85	128.293	28.166	28.065	1.00	55.47	H	
	ATOM	2311	·C	ARG	85	132.670	29.752	34.912	1.00	40.27	H	
	MOTA	2312	0 .	ARG	85	132.430	30.939	34.669	1.00	37.17	H	
	MOTA	2313	N	MET	86	133.645	29.350	35.722	1.00	35.41	H	· ·
	ATOM	2314	CA	MET	86	134.518	30.288	36.412	1.00	32.72	H	1
	ATOM	2315	CB	MET	86	134.974	29.684	37.733	1.00	38.34	H	
	ATOM	2316	CG	MET	86	134.091	28.551	38.215	1.00	45.32	H	
	ATOM	2317	SD	MET	86	133.310	28.856	39.804	1.00	63.97	H	r
	ATOM	2318	CE	MET	86	133.680	30.599	40.068	1.00	45.50	H	
	MOTA	2319	C	MET	86	135.733	30.691	35.592	1.00	33.88	H	
	ATOM	2320	0	MET	86	136.097	30.018	34.627	1.00	28.01	H	
	ATOM	2321	N	THR	87	136.357	31.794	3,5.996	1.00	37.82	H	
	ATOM	2322	CA	THR	87	137.525	32.330	35.310	1.00	39.63	H	4
	MOTA	2323	CB	THR	87	137.081	33.070	34.035	1.00	31.11	H	
	MOTA	2324	OG1	THR	87	136.455	32.132	33.153	1.00	44.08	H	
	MOTA	2325	CG2	THR	87	138.263	33.706	33.324	1.00	41.18	H	

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	ATOM	2326	,C	THR	87	138.299	33.282	36.232	1.00	49.08	\mathbf{H}
	ATOM	2327	0	THR	87	137.797	33.684	37.278	1.00	56.80	H
	ATOM	2328	N	SER	88.	139.523	33.634	35.845	1.00	59.16	H
	ATOM	2329	CA	SER	88	140.362	34.539	36.633	1.00	63.45	H
	ATOM	2330	CB	SER	88	141.693	34.780	35.911	1.00	64.98	H
	ATOM.	2331	OG	SER ···	88	142.614	33.729	36.165	1.00	44.05	H
	ATOM	2332	C	SER	88	139.672	35.878	36.897	1.00	61.47	H
	ATOM	2333	0	SER	88,	140.291	36.838	37.356	1.00	63.13	H
	ATOM	2334	N	GLU	89	138.384	35.928	36.586	1.00	61.96	H
	ATOM	2335	CA	GLU	89	137.567	37.114	36.791	1.00	60.40	H
	ATOM	2336	CB	GLU	89	136.888	37.517	35.483	1.00	58.39	H
	ATOM	2337	CG	GLU	89	136.045	36.410	34.861	1.00	65.30	H
	ATOM	2338	CD	GLU	89	134.607	36.832	34.614	1.00	74.02	H
	ATOM	2339	OE1	GLU	89	134.227	36.969	33.430	1.00	59.34	H
	MOTA	2340	OE2	GLU	89	133.858	37.028	35.604	1.00	71.55	H
	ATOM	2341	C	GLU	89	136.518	36.725	37.822	1.00	58.77	H
	ATOM	2342	0	GLU	89	135.492	37.388	37.971	1.00	54.85	H
	MOTA	2343	N	ASP	90	136.788	35.624	38.514	1.00	59.98	H
	ATOM	2344	CA	ASP	90	135.898	35.102	39.544	1.00	62.69	H
	ATOM	2345	CB	ASP	90	135.475	33.664	39.211	1.00	63.78	H
	ATOM	2346	CG	ASP	90	134.268	33.601	38.293	1.00	63.07	H
	MOTA	2347	OD1	ASP	90	133.728	32.488	38.109	1.00	51.98	H
	MOTA	2348	OD2	ASP	90	133.864	34,.653	37.757	1.00	64.25	H
	MOTA	2349	C	ASP	90	136.653	35.105	40.867	1.00	58.67	H
	ATOM	2350	0	ASP	90	136.052	35.098	41.939	1.00	60.42	H
	ATOM	2351	N	SER	91	137.979	35.102	40.783	1.00	57.82	H
	MOTA	2352	CA	SER	91	138.806	35.113	41.978	1.00	51.69	H
	ATOM	2353	CB	SER	91	140.285	35.096	41.597	1.00	44.52	H
	MOTA	2354	OG	SER	91	140.598	33.935	40.846		46.65	H
	MOTA	2355	C	SER	91	138.487	36.362	42.787	1.00	53.31	H
	MOTA	2356	0	SER	91	138.881	37.471	42.427	1.00	45.71	H
	MOTA	2357	N	ALA	92	137.755	36.167	43.877	1.00	53.93	H
	MOTA	2358	CA	ALA	92	137.356	37.257	44.755	1.00	50.72	H
	ATOM	2359	CB	ALA	92	136.133	37.967	44.177	1.00	48.61	H
	MOTA	2360	C	ALA	92	137.045	36.691	46.143		46.86	H
1	MOTA	2361	0	ALA	92	137.638	35.690	46.545	1.00	49.03	H
ı	MOTA	2362	N	VAL	93	136.116	37.313	46.868	1.00	46.02	H
	ATOM	2363 .	CA	VAL ·	93	135.775	36.842	48.207	1.00	44.17	H
	MOTA	2364	CB	VAL	93	136.116	37.909	49.272		39.83	H
	MOTA	2365		VAL	93	136.006		50.663		31.85	H
	MOTA	2366	CG2		93	137.523		49.049		37.20	H
	MOTA	2367	C	VAL	93	134.330	36.371	48.439		45.91	H
48	ATOM	2368	0		93	134.092		49.301		48.37	H
	ATOM	2369	N	TYR	94	133.373	36.916	47.691		38.60	H
	ATOM	2370	CA	TYR	94	131.963	36.524	47.825	•	49.33	H
	ATOM	2371	CB	TYR	94	131.706		47.125		40.10	Н
	ATOM	2372	CG	TYR	94	132.160	35.137	45.692		31.43	H
	ATOM	2373	CD1		94	131.372				29.40	H
	ATOM	2374		TYR	94	131.758	35.556	•		41.76	H
	ATOM	2375	CD2		94	133.355	34.512	45.346	1.00	33.02	H
	ATOM	2376	CE2	TYR	94	133.750	34.402	44.025		31.73	
	ATOM	2377	CZ	TYR	94	132.949	34.922	43.028		46.94	H
	ATOM	2378	OH	TYR	94	133.336	34.796	41.711	Τ.00	62.64	H

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ATOM	2379	C	TYR	94	131.450	36.407	49.267	1.00 50.08	H
MOTA	2380	, O ,	TYR	94	131.708	35.413	49.953	1.00 34.70	H
MOTA	2381	N	PHE	.95	130.688	37.408	49.703	1.00 50.03	H
MOTA	2382	CA	PHE	95	130.140	37.431	51.051	1.00 34.71	H
MOTA	2383	CB	PHE	95	130.292	38.814	51.671	1.00 32.84	H
ATOM	2384	CG	PHE	95	131.646	39.077	52.243	1.00 19.95	H
MOTA	2385	CD1	PHE	95	131.966	38.638	53.516	1.00 6.35	H
ATOM	2386	CD2	PHE	95	132,600	39.780	51.508	1.00 14.02	H
MOTA	2387	CE1	PHE	95	133.219	38.892	54.057	1.00 29.11	H
MOTA	2388	CE2	PHE	95	133.849	40.037	52.041	1.00 21.81	H
MOTA	2389	CZ	PHE	95	134.162	39.592	53.321	1.00 20.98	H
ATOM	2390	C	PHE	95 ·	128.678	37.082	51.077	1.00 37.58	H
ATOM	2391	0	PHE	95	127.941	37.378	50.146	1.00 40.29	H
ATOM	2392	N	CYS	96	128.272	36.455	52.168	1.00 47.35	H
MOTA	2393	CA	CYS	96	126.888	36.080	52.375	1.00 48.56	H
ATOM	2394	C	CYS	96	126.368	37.062	53.415	1.00 47.93	H
MOTA	2395	0	CYS	96	127.035	37.326	54.420	1.00 49.37	H
ATOM	2396	CB	CYS	96	126.796	34.652	52.911	1.00 45.82	H
ATOM	2397	SG	CYS	96	125.140	34.190	53.511	1.00 75.54	H
ATOM	2398	N	THR	97	125.188	37.614	53.168	1.00 37.05	H
ATOM	2399	CA	THR	97	124.595	38.575	54.086	1.00 35.84	H
ATOM	2400	CB	THR	97	125.127	40.008	53.807	1.00 33.55	·H
ATOM	2401	OG1	THR	97	124.832	40.851	54.922	1.00 24.79	H
MOTA	2402	CG2	THR	97	124.517	40.584	52.542	1.00 23.01	H
MOTA	2403	C	THR	97	123.085	38.518	53.931	1.00 34.60	H
MOTA	2404	0	THR	97	122.584	37.860	53.026	1.00 34.26	H
ATOM	2405	N	ARG	98	122.356	39.192	54.814	1.00 46.98	\mathbf{H}
ATOM	2406	CA	ARG	98	120.896	39.158	54.752	1.00 49.01	H
MOTA	2407	CB	ARG	98	120.352	38.157	55.795	1.00 38.44	H
MOTA	2408	CG	ARG	98	119.596	38.781	56.963	1.00 40.81	H
ATOM	2409	CD	ARG	98	120.319	38.594	58.296	1.00 27.38	H
MOTA	2410	NE	ARG	98	119.849	39.546	59.307	1.00 53.08	H
MOTA	2411	CZ	ARG	98	119.540	39.230	60.563	1.00 40.53	H
MOTA	2412	NH1	ARG	98	119.651	37.977	60.980	1.00 58.43	H
MOTA	2413	NH2	ARG	98	119.113	40.167	61.403	1.00 33.33	H
MOTA	2414	C	ARG	98	120.229	40.507	54.938	1.00 39.44	· H
MOTA	2415	0	ARG	98	120.740	41.377	55.637	1.00 41.38	H
MOTA	2416	N	SER	99	119.079	40.666	54.296	1.00 35,04	H
MOTA	2417	CA	SER	99	118.299	41.889	54.388	1.00 24.81	H
MOTA	2418	CB	SER	99	117.920	42.396	53.004	1.00 14.04	H
ATOM	2419	OG	SER	99	117.671	43.780	53.039	1.00 29.22	H
ATOM	2420	С	SER	99	117.050	41.455	55.106	1.00 28.87	H
ATOM	2421	0	SER	99	116.660	40.294	55.009	1.00 36.12	H
MOTA	2422	N	HIS	100	116.418	42.367	55.829	1.00 34.54	H
ATOM	2423	CA	HIS	100	115.209	41.998	56.541	1.00 40.60	H
MOTA	2424	CB	HIS	100	114.976	42.943	57.714	1.00 35.00	H
ATOM	2425	CG	HIS	100	113.731	42.641	58.492	1.00 48.41	, H
MOTA	2426	, CD2	HIS	100	113.141	41.463	58.812	1.00 45.56	H
MOTA	2427	ND1	HIS	100	112.947	43.625	59.057	1.00 32.49	H
MOTA	2428	CE1	HIS	100	111.930	43.069	59.687	1.00 29.00	H
MOTA	2429	NE2	HIS	100	112.023	41.759	59.557	1.00 33.71	H
MOTA	2430	C	HIS	100	114.037	42.072	55.584	1.00 41.32	H
MOTA	2431	0	HIS	100 .	113.824	43.110	54.964	1.00 48.72	\mathbf{H}

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MOTA	2432 -	Ň	TYR	101	ı	113.295	40.976	55.438	1.00	35.01	H
MOTA	2433	CA	TYR	101		112.136	41.001	54.551	1.00	39.86	H
MOTA	2434	CB	TYR	101		111.509	39.606	54.408	1.00	26.52	H
MOTA	2435	CG	TYR	101		110.507	39.496	53.267	1.00	26.05	H
MOTA	2436	CD1	TYR	101		110.933	39.404	51.945	1.00	40.86	H
MOTA	2437	CE1	TYR	101		110.024	39.324	50.885	1.00	27.58	H
MOTA	2438	CD2	TYR	101		109.135	39.502	53.507	1.00	33.96	H
MOTA	2439	CE2	TYR	101		108.216	39.422	52.450	1.00		H
MOTA	2440	CZ	TYR	101		108.673	39.336	51.145	1.00	27.74	H
MOTA	2441	OH	TYR	101		107.779	39.275	50.100	1.00	40.21	H
MOTA	2442	C	TYR	101		111.167	41.950	55.247	1.00	55.50	H
MOTA	2443	0	TYR	101		111.013	41.892	56.470	1.00		. H
MOTA	2444	N	GLY	102		110.525	42.828	54.482	1.00		H
ATOM	2445	CA	GLY	102	ч	109.611	43.790	55.079	1.00	, "	H
ATOM	2446	, C	GLY	102	4	110.364	45.094	55.237	1.00		H
MOTA	2447	0	GLY	102		110.169	46.028	54.464	1.00		H
ATOM	2448	N	LEU	103		111.229	45.155	56.243	1.00	31.80	H
ATOM	2449	CA	LEU	103		112.062	46.331	56.475	1.00	34.98	H
MOTA	2450	CB	LEU	103		112.270	46.554	57.975	1.00	47.24	H
ATOM	2451	CG	LEU	103		111.258		58.750		56.12	H
ATOM	2452	CD1	LEU	103		109.959	47.593	57.956	1.00		H
ATOM	2453	CD2	LEU	103		110.993	46.730	60.092	1.00	44.52	H
ATOM	2454	C	LEU	103	K	113.394	46.019	55.807	1.00	31.85	H
ATOM	.2455	0	LEU	103		114.392	45.736	56.471	1.00	32.76	H
ATOM	2456	N	ASP	104		113.368	46.045	54.477	1.00	33.42	H
ATOM	2457	CA	ASP	104		114.512	45.757	53.625	1.00	20.79	H
ATOM	2458	CB	ASP	104		113.992	45.202	52.295	1.00	32.02	H
ATOM	2459	CG	ASP	104		115.093 114.753	44.901	51.298 50.136	1.00	55.62 38.63	H
ATOM	2460	OD1	ASP	104	,	116.286	44.985	51.663	1.00	61.09	H
ATOM ATOM	2461 2462	OD2	ASP ASP	104 104		115.255	47.067	53.415	1.00		H H
ATOM	2463	0	ASP	104		115.233	47.775	52.440	1.00	33.69	H
ATOM	2464	N	TRP	105	,	116.148	47.775	54.346	1.00	37.55	H
ATOM	2465	CA	TRP	105		116.907	48.628	54.288	1.00	32.28	H
ATOM	2466	CB	TRP	105		116.599	49.484	55.518	1.00	42.44	H
ATOM	2467	CG	TRP	105		115.123	49.751	55.717	1.00	44.69	H
ATOM	2468	CD2	TRP	105		114.456	50.028	56.955	1.00	43.59	H
ATOM	2469	CE2		105		113.091	50.217	56.662	1.00	39.38	H
ATOM	2470	CE3	TRP	105		114.887	50.136	58.285	•	53.16	H
ATOM	2471	CD1		105		114.157	49.780	54.751		25.93	H
ATOM	2472	NEL	TRP	105		112.942	50.059	,		37.01	Н
ATOM	2473	CZ2	TRP	105		112.144	50.507	57.650		45.54	H
MOTA	2474	CZ3	TRP	105		113.945	50.425	59.270		48.69	
ATOM	2475	CH2	TRP	105		112.588	50.609	58.945		55.24	Н
ATOM	2476	C	TRP	105		118.405	48.421	54.187	1.00	40.80	H
ATOM	2477	0	TRP	105		119.063	49.042	53.352	1.00	47.85	H
ATOM	2478	N	ASN	106		118.952	47.556	55.038	1.00	49.48	H
MOTA	2479	CA	ASN	106		120.389	47.305	55.013	1.00	46.39	H
ATOM	2480	CB	ASN	106		121.103	48.280	55.951	1.00	36.85	Н
ATOM	2481	CG	ASN	106		120.869	47.961	57.408	1.00	28.91	H
MOTA	2482	OD1	ASN	106		119.909	48.434	58.013	1.00	32.97	H
ATOM	2483	ND2	ASN	106		121.744	47.152	57.981	1.00	41.71	H
MOTA	2484	C	ASN	106		1,20.786	45.877	55.363	1.00	48.25	H
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ATOM	2485	0	ASN	106	119.950	45.059	55.760	1.00 46.92	H
ATOM	2486	N	PHE	107	122.079	45.602	55.202	1.00 47.37	H
ATOM	2487	CA	PHE	1.07	122.665	44.294	55.489	1.00 47.06	H
MOTA	2488	CB	PHE	107	123.589	43.862	54.341	1.00 51.22	H
MOTA	2489	CG	PHE	107	123.004	44.052	52.954	1.00 36.58	H
ATOM	2490	CD1	PHE	107	121.628	44.053	52.737	1.00 43.99	H
ATOM	2491	CD2	PHE	107	123.847	44.180	51.851	1.00 35.28	H
MOTA	2492	CE1	PHE	107	121.107	44.175	51.449	1.00 41.51	H
ATOM	2493	CE2	PHE	107	123.334	44.301	50.561	1.00 20.31	H
ATOM	2494	CZ	PHE	107	121.965	44.296	50.362	1.00 40.17	H
ATOM	2495	C	PHE	107	123.479	44.386	56.787	1.00 45.87	H
MOTA	2496	0	PHE	107	124.641	44.805	56.765	1.00 38.80	H
MOTA	2497	\mathbf{N}	ASP	108	122.874	43.982	57.905	1.00 44.31	H
MOTA	2498	CA	ASP	108	123.528	44.053	59.215	1.00 40.48	H
MOTA	2499	CB	ASP	108	122.479	44.243	60.325	1.00 54.96	H
MOTA	2500	CG	ASP	108	121.048	44.057	59.833	1.00 66.26	H
MOTA	2501	OD1	ASP	108	120.304	45.059	59.790	1.00 56.03	H
MOTA	2502	OD2	ASP	108	120.664	42.914	59.494	1.00 63.18	H
ATOM	2503	C	ASP	108	124.445	42.889	59.600	1.00 27.53	H
MOTA	2504	0	ASP	108	125.418	43.077	60.328	1.00 16.20	H
MOTA	2505	N	VAL	109	124.133	41.690	59.128	1.00 18.58	H
MOTA	2506	CA	VAL	109	124.946	40.527	59.458	1.00 20.11	. H
MOTA	2507	CB	VAL	109	124.072	39.410	60.037	1.00 25.57	H
ATOM	2508	CG1	VAL	109	124.936	38.353	60.691	1.00 22.40	H
MOTA	2509	CG2	VAL	109	123.098	39.998	61.038	1.00 21.93	H
MOTA	2510	C	VAL	109	125.704	39.984	58.246	1.00 26.64	H
MOTA	2511	0	VAL	109	125.110	39.594	57.248	1.00 34.79	H
ATOM	2512	N	TRP	110	127.023	39.949	58.336	1.00 27.30	H
ATOM	2513	CA	TRP	110	127.818	39.459	57.229	1.00 27.28	H
ATOM	2514	CB	TRP	110	128.834	40.519	56.810	1.00 33.78	H
ATOM	2515	CG	TRP	110	128.248	41.738	56.167	1.00 36.21	H H.
ATOM	2516	CD2	TRP	110	128.440	42.162	54.813	1.00 25.48 1.00 33.24	H.
ATOM	2517	CE2	TRP	110	127.801 129.097	43.411 41.609	54.669 53.711	1.00 33.24	H
MOTA	2518	CE3	TRP	110	127.511	42.715	56.770	1.00 42.55	H
ATOM	2519	CD1	TRP	110 110	127.236	43.728	55.879	1.00 42.33	H
ATOM	2520	NE1	TRP TRP	110	127.795	44.115	53.467	1.00 36.00	H
ATOM	2521	CZ2	TRP	110	129.096	42.314	52.511	1.00 25.21	H
ATOM ATOM	2522 2523	CZ3 CH2	TRP	110	128.449	43.553	52.402	1.00 36.50	H
ATOM	2524 2524	C	TRP	110	128.566	38.187	57.601	1.00 29.69	H
ATOM	2525	0	TRP	110	128.946	37.993	58.753	1.00 39.20	H
ATOM	2526	N	GLY	111	128.774	37.317	56.621	1.00 26.69	Н
ATOM	2527	CA	GLY	111	129.523	36.110	56.880	1.00 15.66	H
ATOM	2527 2528	CA	GLY	111	130.988	36.505	56.847	1.00 32.31	H
ATOM	2529	0	GLY	111	131.327	37.622	56.451	1.00 24.60	Н
ATOM	2530	N	ALA	112	131.867	35.604	57.261	1.00 41.72	H
ATOM	2531	CA	ALA	112	133.287	35.907	57.249	1.00 41.34	H
ATOM	2531	CB	ALA	112	134.033	34.911	58.119	1.00 39.24	H
ATOM	2532	C	ALA	112	133.857	35.896	55.826	1.00 45.93	Н
ATOM	2534	0	ALA	112	134.902	36.492	55.568	1.00 49.85	H
ATOM	253 4 2535	N	GLY	113	133.178	35.217	54.906	1.00 45.09	H
ATOM	2535 2536	CA	GLY	113	133.665	35.161	53.538	1.00 44.98	H
ATOM	2537	CA	GLY	113	134.180	33.798	53.099	1.00 44.48	H
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MOTA	2538	Ο,,	GLY	. 113	ı	134.273	32.862	53.894	1.00	40.99	H
MOTA	2539	N	THR	114	•	134.519	33.690	51.819	1.00	44.31	H
MOTA	2540	CA	THR	114		135.019	32.446	51.242	1.00	31.88	$^{\circ}$ H
MOTA	2541	CB	THR	114	×	133.845	31.530	50.772	1.00	20.38	H
MOTA	2542	OG1	THR	114		133.279	30.861	51.900	1.00	35.87	H
ATOM	2543	CG2	THR	114		134.328	30.478	49.789	1.00	32.39	H
MOTA	2544	C	THR	114		135.865	32.814	50.032	1.00	33.60	H
MOTA	2545	0	THR	114	ı	135.325	33.054	48.953	1.00	42.98	H
ATOM	2546	N	THR	115		137.182	32.880	50.208	1.00	35.92	H
ATOM	2547	CA	THR	115		138.055	33.208	49.089	1.00	33.21	H
ATOM	2548	CB	THR	115		139.525	33.317	49.499	1.00	43.78	H
ATOM	2549	OG1	THR	115		139.649	34.185	50.632	1.00	41.45	H
MOTA	2550	CG2	THR	115		140.351	33.867	48.332	1.00		H
MOTA	2551	C	THR	115		137.938	32.100	48.059	1.00		
MOTA	2552	0	THR	115		137.823	30.918	48.406	1.00	28.11	H
ATOM	2553	N	VAL	116		137.958	32.490	46.791	1.00		H
ATOM	2554	CA	VAL	116		137.840	31.537	45.708	1.00	40.64	H
ATOM	2555	CB	VAL	116		136.443	31.616	45.051	1.00	41.04	H
ATOM	2556	CG1	VAL	116		136.337	30.599	43.931	1.00	35.25	H
ATOM	2557	CG2	VAL	116		135.362	31.359	46.096	1.00	33.28	H
ATOM	2558	C	VAL	116		138.899	31.816	44.661	1.00	43.76	H
ATOM	2559	0	VAL	116		139.009	32.929	44.146	1.00		H
ATOM	2560	N	THR	117	£	139.683	30.791	44.354	1.00		H
ATOM	2561	CA	THR	117		140.740	30.919	43.370	1.00	40.89	H
ATOM	2562	CB	THR	117		142.095	30.552	43.969	1.00	38.40	H
MOTA	2563	OG1	THR	117		142.320	31.340	45.145	1.00	36.59	H
ATOM	2564	CG2	THR	117		143.205	30.810	42.966	1.00	32.70	H
MOTA	2565	C	THR	117		140.449	30.001		1.00	38.02	H
MOTA	2566. 2567	O	THR	117		139.802 140.928	28.971 30.386	42.357 41.031	1.00	37.58 45.45	H
ATOM ATOM	2567 2568	N CA	VAL VAL	118 118		140.705	29.597	39.838	1.00	47.20	Н
ATOM	2569	CB	VAL	118		140.703	30.481	38.694	1.00	54.07	H
ATOM	2570	CG1	VAL	118		138.698	30.704	38.844		40.64	H
ATOM	2571	CG2	VAL	118		140.942	31.807	38.700	1.00		H
ATOM	2572	C	VAL	118		141.973	28.890	39.400		42.28	H
ATOM	2573	0	VAL	118		141.946	27.706	39.060	1.00	42.04	H
ATOM	2574	N	SER	119		143.081	29.622	39.415		40.12	H
ATOM	2575	CA	SER-			144.381	29.089	39.015	1.00	48.99	Н
ATOM	2576	CB	SER	119		145.469	29.569	39.983		49.51	H
MOTA	2577	OG	SER	119		146.419	30.398	39.331	1.00	31.69	Н
MOTA	2578	C	SER	119		144.418	27.563	38.929	1.00	49.87	H
ATOM	2579	0	SER	119		144.028	26.856	39.870	1.00	42.52	H
MOTA	2580	N	SER	120		144.887	27.067	37.787	1.00	55.96	H
MOTA	2581	CA	SER	120		144.996	25.633	37.540	1.00	53.80	H
ATOM	2582	CB	SER	120		144.774	25.334	36.050	1.00	57.59	H
ATOM	2583	OG	SER	120		145.785	25.919	35.239	1.00	55.34	H
MOTA	2584	C	SER	120		146.377	25.145	37.965	1.00	53.97	H
MOTA	2585	0	SER	120		146.879	24.149	37.447	1.00	49.63	H
ATOM	2586	N	ALA	121	•	146.974	25.858	38.919	1.00	62.49	H
MOTA	2587	CA	ALA	121		148.307	25.544	39.445	1.00	58.34	H
MOTA	2588	CB	ALA	121	•	148.830	26.714	40.278	1.00	52.59	H
MOTA	2589	C	ALA	121	*	148.333	24.268	40.284	1.00	54.04	H
ATOM	2590	0	ALA	121		147.318	23.584	40.432	1.00	56.38	H

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ATOM	2591	N	LYS	122	149.498	23.951	40.841	1.00	48.35	-	H
ATOM	2592	CA	LYS	122	149.624	22.750	41.649	1.00	46.60		H
ATOM	2593	CB	LYS	122	150.912	21.998	41.318	1.00	51.72	2	H
ATOM	2594	CG	LYS	122	150.682	20.565	40.843	1.00	51.16		H
ATOM	2595	CD	LYS	122	150.117	19.675	41.948	1.00	40.43		H
MOTA	2596	CE.	LYS	122	151.191	18.754	42.525	1.00	52.69		H
MOTA	2597	NZ	LYS	122	150.980	17.320	42.166	1.00	52.23		H
ATOM	2598	C	LYS	122	149.577	23.043	43.133	1.00	52.24		H
ATOM	2599	0	LYS	122	150.258	23.933	43.644	1.00	51.54		H
MOTA	2600	N	THR	123	148.758	22.255	43.811	1.00	58.75		H
ATOM	2601	CA	THR	123	148.562	22.363	45.249	1.00	59.16		H
MOTA	2602	CB	THR	123	147.422	21.459	45.722	1.00	70.62		H
ATOM	2603	OG1	THR	123	146.234	21.774	44.989	1.001	100.00		H
ATOM	2604	CG2	THR	123	147.174	21.644	47.216	1.00	71.56		H
MOTA	2605	C	THR	123	149.851	21.904	45.913	1.00	59.76		H
ATOM	2606	0	THR	123	150.327	20.797	45.654	1.00	51.50		H
MOTA	2607	N	THR	124	150.430	22.671	46.957	1.00	60.58		H
MOTA	2608	CA	THR	124	151.805	22.409	47.339	1.00	54.63		H
MOTA	2609	CB.	THR	124	152.776	23.187	46.433	1.00	44.65		H
MOTA	2610	OG1	THR	124	152.458	22.930	45.055	1.00	43.48		H
MOTA	2611	CG2	THR	124	154.207	22.779	46.719	1.00	35.75		H
MOTA	2612	C	THR	124	152.034	22.844	48.776	1.00	61.90		H
ATOM	2613	0	THR	124	151.832	24.005	49.113	1.00	66.47		H
ATOM	2614	N	PRO	125	152.470	21.918	49.644	1.00	63.12		H
MOTA	2615	CD	PRO	125	152.792	20.505	49.387	•	43.60		H
ATOM	2616	CA	PRO	125	152.705	22.286	51.044	1.00	64.11		H
ATOM	2617	CB	PRO	125	153.012	20.956	51.725		53.31	:	H
MOTA	2618	CG	PRO	1	153.525	20.089	50.636		27.09		H
MOTA	2619	C	PRO	125	153.858	23.274	51.141		60.12		H
MOTA	2620	0	PRO	125	154.781	23.255	50.329		49.68	1	H
MOTA	2621	N	PRO	126	153.811	24.153	52.140	1.00	55.19	1	H
ATOM	2622	CD	PRO	126	152.761	24.258	53.169	1.00	61.07		H
MOTA	2623	CA	PRO	126	154.855	25.156	52.333	1.00	47.53		H
ATOM	2624	CB	PRO	126	154.213	26.141	53.296	1.00	49.84		H
MOTA	2625	CG	PRO	126	153.315	25.289	54.118	1.00	73.92		H
ATOM	2626	C	PRO	126	156.155	24.608	52.891	1.00	49.11		H
MOTA	2627	0	PRO	126	156.148	23.695	53.716	1.00	53.71		H
ATOM	2628	N	SER	127	157.266	25.174	52.429		38.85		H
ATOM	2629	CA	SER	127	158.586	24.792	52.913		21.97	*	H
ATOM	2630	CB	SER	127	159.628	24.904	51.798		39.50		H
MOTA	2631	OG	SER	127	159.487	23.866	50.845		52.42		H
ATOM	2632	C	SER	127	158.864	25.826	53.990		33.98	v s	H
ATOM	2633	0	SER	127	159.021	27.008	53.687		34.88		H.
ATOM	2634	N	VAL	128	158.903	25.393	55.243		39.20	-	
ATOM	2635	CA	VAL	128	159.135	26.308	56.353		46.26		H
ATOM	2636	CB	VAL	128	158.247	25.929	57.562		49.37		H H
ATOM	2637	CG1		128	158.162	27.089	58.545	1.00	42.90		H
ATOM	2638	•	VAL	128	156.862	25.538	57.078	1.00	51.53		H
ATOM	2639	C	VAL	128	160.594	26.350	56.794	1.00	37.55 49.56	Ŧ	H
ATOM	2640	O N7	VAL	128	161.183	25.329	57.153	1.00	49.56		H
ATOM	2641	N	TYR	129	161.172	27.545	56.765	1.00			H
ATOM	2642	CA	TYR	129	162.562	27.740	57.150	1.00	44.86		H
ATOM	2643	CB	TYR	129	163.364	28.279	55.969	T.00	35.54		11

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MOTA	2644	CG	TYR	129		163.348	27.402	54.736	1.00 27.5	5 · · ·	H	1		
MOTA	2645	CD1	TYR	129,	:	163.718	26.059	54.800	1.00 42.4	4	H			
ATOM	2646	CE1	TYR	129		163.729	25.256	53.654	1.00 44.4	5	H			•
ATOM	2647	CD2	TYR	129		162.986	27.928	53.497	1.00 28.7	7	H			
ATOM	2648	CE2	TYR	129		162.991	27.135	52.345	1.00 44.20	5	H			
MOTA	2649	CZ	TYR	129		163.363	25.806	52.430	1.00 46.9	5 ·	H			
ATOM	2650	OН	TYR	129		163.366	25.036	51.291	1.00 71.83	L	H			
ATOM	2651	C	TYR	129		162.670	28.722	58.312	1.00 41.49	9	H		**	
MOTA	2652	0	TYR	129		162.195	29.856	58.225	1.00 48.70	5	H			
ATOM	2653	\mathbf{N} .	PRO	130		163.309	28.302	59.415	1.00 46.24	1	H			
ATOM	2654	CD	PRO	130		163.913	26.972	59.604	1.00 58.08	3 ,	H			
ATOM	2655	CA	PRO	130		163.482	29.152	60.597	1.00 40.62	2	H			
ATOM	2656	CB	PRO	130		163.970	28.180	61.661	1.00 49.23	L	H			
ATOM	2657	CG	PRO	130		164.699	27.132	60.872	1.00 50.86	5	H			
ATOM	2658	·C	PRO	130		164.486	30.276	60.359	1.00 42.13	3	H			
ATOM	2659	0	PRO	130		165.506	30.079	59.704	1.00 49.80		H			
MOTA	2660	N	LEU	131		164.195	31.455	60.895	1.00 40.92	2	H			
MOTA	2661	CA	LEU	131		165.081	32.598	60.732	1.00 35.23	3	H			
ATOM	2662	CB	LEU	131		164.319	33.772	60.120	1.00 34.49	€	H)		
MOTA	2663	CG	LEU	131		163.916	33.644	58.652	1.00 34.92	2	H			
ATOM	2664	CD1		131		163.135	34.878	58.245	1.00 11.53	L	H			
MOTA	2665	CD2	LEU	131		165.144	33.483	57.781	1.00 26.6	7	H		•	
ATOM	2666	C	LEU	131		165.666	33.014	62.077	1.00 40.36	5	H			
ATOM	2667	0	LEU	131		164.956	33.557	62.927	1.00 46.95	5	H			
ATOM	2668	N	ALA	132		166.956	32.755	62.263	1.00 56.70) -	H			
ATOM	2669	CA	ALA	132		167.632	33.110	63.507	1.00 56.73	<u>.</u> .	H·			
ATOM	2670	CB	ALA	132	•	168.300	31.886	64.096	1.00 57.53	3	H			
ATOM	2671	C	ALA	132		168.662	34.210	63.268	1.00 55.87	7	H			
ATOM	2672	0	ALA	132		169.276	34.279	62.204	1.00 54.54	Ł	H	"	:	
ATOM	2673	N	PRO	133		168.864	35.091	64.262	1.00 57.72	2	H			
MOTA	2674	CD	PRO	133	e	168.161	35, 065	65.557	1.00 47.07	7	H			
ATOM	2675	CA	PRO	133	ı	169.815	36.206	64.187	1.00 60.50) , '	Ħ		'	
ATOM	2676	CB	PRO	133		169.496	37.030	65.431	1.00 59.11	L	H			
ATOM	2677	CG	PRO	133		168.946	36.033	66.393	1.00 46.85	5	H			
ATOM	2678	C	PRO	133		171.285	35.780	64.154	1.00 64.47	7	H			**
ATOM	2679	0	PRO	133		171.743	35.030	65.021	1.00 63.82	2	H			
MOTA	2680	$\mathbf{N}_{\dot{i}}$	GLY	134	i	172.021	36.276	63.161	1.00 66.38	3	H			
ATOM	2681	CA	GLY	134		173.429	35.937	63.030	1.00 54.50)	H			4
MOTA	2682	C	GLY	134		174.356	36.531	64.074	1.00 60.13	3	H			
ATOM	2683	0	GLY	134		175.515	36.851	63.795	1.00 70.75	5	H	ė.		
ATOM	2684	N	SER	135		173.893	36.652	65.276	1.00 74.93	}	H			
ATOM	2685	CA	SER	135		174.743	37.216	66.319	1.00 86.16	5	H			
MOTA	2686	CB	SER	135		176.038	36.396	66.439	1.00 90.22	?	H .		y.	
ATOM	2687	OG	SER	135		176.965	36.773	65.426	1.00100.00) ' ,	H.			
ATOM	2688	C	SER	135		175.096	38.660	65.950	1.00 88.57	7	H			
ATOM	2689	O .	SER	135		176.088	38.928	65.255	1.00 77.68	3	H			
MOTA	2690	N	ALA	136		174.255	39.552	66.431	1.00 94.60)	H			
MOTA	2691	CA	ALA	. 136		174.413	40.992	66.206	1.00 96.15		H			
MOTA	2692	CB	ALA	136		174.299	41.304	64.714	1.00 91.75		H			
MOTA	2693	C	ALA	136		173.334	41.759	66.962	1.00 99.99)	H	"		
ATOM	2694	0	ALA	136		172.158	41.398	66.918	1.00 99.98		H			
ATOM	2695	N	ALA	137		173.740	42.818	67.655	1.00 99.99		H			
ATOM	2696	CA	ALA	137		172.802	43.637	68.417	1.00100.00)	H		_	
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ATOM	2697	CB	ALA	137		173.565	44.631	69.285	1.00	89.73	•	H
ATOM	2698	C.	ALA	137		171.860	44.377	67.474	1.00	99.97		H
ATOM	2699	0	ALA	137		172.119	45.518	67.094	1.00	99.95	•	H
MOTA	2700	N	GLN	138		170.768	43.718	67.103	1.00	99.99		H
ATOM	2701	CA	GLN	138		169.788	44.308	66.198	1.00	99.99		H
ATOM	2702	CB	GLN	138		168.740	43.264	65.804	1.00	92.32		H
ATOM	2703	CG	GLN	138		167.946	42.702	66.972	1.00	80.27		H
ATOM	2704	CD	GLN	138		166.461	42.627	66.679	1.00	62.10		H
ATOM	2705	OE1	GLN	138		166.051	42.463	65.530	1.00	72.23		H
ATOM	2706	NE2	GLN	138		165.646	42.749	67.720	1.00	47.02		H
ATOM	2707	С	GLN	138		169.100	45.522	66.818	1.00	99.97		H
ATOM	2708	0	GLN	138		168.850	46.516	66.136	1.00	99.97		H
ATOM	2709	N	THR	139		168.797	45.438	68.116	1.00	99.99		H
ATOM	2710	CA	THR	139	ŧ	168.138	46.530	68.810		100.00		H
ATOM	2711	CB	THR	139		166.629	46.520	68.570		100.00		H
ATOM	2712	OG1	THR	139		166.068	45.306	69.085	1.00			H
ATOM	2713	CG2	THR	139		166.326	46.637	67.084	1.00	99.99	:	H
ATOM	2714	C	THR	139		168.421	46.461	70.301	1.00	99.99		H
ATOM	2715	0	THR	139		167.865	45.622	71.014	1.00	99.98		H
ATOM	2716	Ŋ	ASN	140		169.282	47.359	70.792	1.00	99.98		H
ATOM	2717	CA	ASN	140		169.654	47.435	72.187	1.00	96.92		H
ATOM	2718	CB	ASN	140		168.714	48.381	72.927	1.00	94.82		H
ATOM	2719	CG	ASN	140		168.783	49.786	72.357	1.00	91.71		H
ATOM	2720	OD1	ASN	140	4	169.866	50.280	72.032	1.00	88.37		H
	2721	ND2	ASN	140		167.633	50.433	72.229	1.00	91.05	•	H
ATOM		C		•		167.033	46.052	72.801	1.00	93.43	,	H
ATOM	2722		ASN	140		170.715	45.321	72.647	1.00	83.04		H
ATOM	2723	O NT	ASN	140		168.684	45.691	73.529	1.00	91.74		H
ATOM	2724	N	SER	141			44.391	74.200	1.00	78.99		H
MOTA	2725	CA	SER	141		168.629	r	75.629	1.00	69.11		H
ATOM	2726	CB	SER	141		168.101	44.544					H
ATOM	2727	OG	SER	141		166.899	45.297	75.639	1.00	60.50		Н
ATOM	2728	C	SER	141		167.726	43.431	73.432	1.00	75.37		H
ATOM	2729	O	SER	141		168.173	42.413	72.896	1.00	88.08		H
ATOM	2730	N	MET'	142		166.479	43.787	73.391	1.00	59.56		
MOTA	2731	CA	MET	142		165.449	42.970	72.766	1.00	44.97		H
ATOM	2732	CB	MET	142	• :	164.206	43.807	72.516	1.00	56.70	•	H
ATOM	2733	CG	MET	142		163.645	44.397	73.800	1.00	86.09		H
ATOM	2734	SD	MET	142	r	162.177	45.354	73.535	1.00	99.97		H
ATOM	2735	CE	MET	142		162.239	46.814	74.546	1.00	99.42		H
ATOM	2736	C	MET	142	•	165.871	42.372	71.432	1.00	32.94		H
ATOM	2737	0	MET	142		166.780	42.880	70.772	1.00	33.63		H
MOTA	2738	N	VAL	143		165.183	41.304	71.027	1.00	27.18		H
MOTA	2739	CA.	VAL	143		165.501	40.615	69.779	1.00	24.76		H
ATOM	2740	CB	VAL	143		166.197	39.272	70.065	1.00	10.57		H
ATOM	2741	CG1	VAL	143		165.186	38.268	70.594	1.00	34.15	:	H
MOTA	2742	CG2	VAL	143		166.872	38.750	68.800	1.00	21.19		H
MOTA	2743	C	VAL	143		164.299	40.345	68.871	1.00	32.37		H
MOTA	2744	0	VAL	143	* 4	163.150	40.451	69.293	1.00	31.65	•	H
MOTA	2745	N	THR	144		164.588		67.623	1.00	32.76		H
MOTA	2746	CA	THR	144		163.561	39.686	66.630	1.00	32.18		H
ATOM	2747	CB	THR	144		163.459	40.810	65.580	1.00	23.79		H
MOTA	2748	OG1	THR	144		162.934	41.991	66.196	1.00	53.98		H
MOTA	2749	CG2	THR	144		162.543	40.394	64.436	1.00	20.69		H

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ATOM	2750	C	THR	144	163.855	38.384	65.891	1.00	39.99	H
ATOM	2751	0	THR	144	164.958	38.178	65.384	1.00	46.16	. H
MOTA	2752	N	LEU	145	162.858	37.507	65.830	1.00	32.72	H
MOTA	2753	CA	LEÙ	145	163.004	36.237	65.138	1.00	13.00	H
ATOM	2754	CB	LEU	145	162.645	35.082	66.062	1.00	22.16	H
ATOM	2755	CG	LEU	145	163.748	34.615	67.003	1.00	24.64	H
MOTA	2756	CD1	LEU	145	163.529	35.237	68.3 ⁷ 6	1.00	21.35	H
MOTA	2757	CD2	LEU	145	163,736	33.095	67.084	1.00	18.63	. H
MOTA	2758	, C ,	LEU	145	162.064	36.220	63.948	1.00	24.06	H
MOTA	2759	0	LEU	145	161.188	37.073	63.831	1.00	32.59	H
MOTA	2760	N	GLY	146	162.244	35.240	63.072	1.00	32.97	H
MOTA	2761	CA	GLY	146	161.397	35.153	61.903	1.00	32.08	H
MOTA	2762	C	GLY	146	161.254	33.741	61.381	1.00	29.89	H
MOTA	2763	0	GLY	146	161.995	32.845	61.778	1.00	19.61	H
MOTA	2764	N	CYS	147	160.283	33.553	60.499	1.00	39.08	H
MOTA	2765	CA	CYS	147	160.023	32.258	59.885	1.00	38.87	H
MOTA	2766	C	CYS	147	159.696	32.518	58.425	1.00	30.42	H
MOTA	2767	0	CYS	147	158.934	33.431	58.109	1.00	37.75	H
MOTA	2768	CB	CYS	147	158.843	31.560	60.574	1.00	55.35	, Н
MOTA	2769	SG	CYS	147	159.313	30.021	61.435	1.00	81.70	H
MOTA	2770	N	LEU	148	160.288	31.730	57.536	1.00	28.82	H
MOTA	2771	CA	LEU	148	160.037	31.891	56.115	1.00	27.56	H
MOTA	2772	CB	LEU	148	161.363	31.967	55.352	1.00	34.75	H
MOTA	2773	CĠ	LEU	148	161.254	32.129	53.831	1.00	34.95	H
MOTA	2774	CD1	LEU	148	160.549	33.425	53.488	1.00	18.93	H
ATOM	2775	CD2	LEU	148	162.636	32.111	53.219	1.00	21.69	H
MOTA	2776	C	LEU	148	159.187	30.737	55.580	1.00	24.86	H
ATOM	2777	0	LEU	148	159.576	29.572	55.663	1.00	30.70	H
ATOM	2778	N	VAL	149	158.020	31.077	55.045	1.00	27.57	H
ATOM	2779	CA	VAL	149	157.091	30.096	54.487	1.00	25.23	H
MOTA	2780	CB	VAL	149	155.658	30.376	54.969	1.00	3.47	H
ATOM	2781	CG1	VAL	149	154.800	29.127	54.827	1.00	25.66	- H
ATOM ·	2782	CG2	VAL	149	155.695	30.830	56.417	1.00	15.58	H
ATOM	2783	C	VAL	149	157.152	30.207	.52.969	1.00	43.19	H
ATOM	2784	0	VAL	149	156.520	31.080	52.375	1.00	55.54	H
ATOM	2785	Ŋ	LYS	150	157.906	29.313	52.341	1.00	45.51	H
ATOM	2786	CA	LYS	150	158.078	29.377	50.897		36.67	H
ATOM	2787	CB	LYS	150	159.572	29.376	50.570	1.00	23.27	H
ATOM	2788	CG	LYS	150	159.950	30.226	49.366	1.00	37.80	H
ATOM	2789	CD	LYS	150	161.441	30.145	49.070		45.44	H
ATOM	2790	CE	LYS	150	161.689	29.729	47.631	1.00		H
ATOM	2791	NZ	LYS	150	163.035	30.147	47.149	1.00	74.67	H
ATOM	2792	C	LYS	150	157.393	28.322	50.047		47.62	H
	2793	0	LYS	150	157.086	27.225	50.503			H
ATOM	2794	N	GLY	151	157.172	28.686	48.789	1.00		H
ATOM	2795	CA	GLY	151	156.562	27.808	47.805		56.42	H
ATOM	2796	C	GLY	151	155.344	26.981	48.176		65.95	H
MOTA	2797	0	GLY	151	155.404	25.751	48.146		83.19	H
ATOM	2798	N	TYR	152	154.238	27.641	48.522		68.59	H
ATOM	2799	CA	TYR	152	153.018	26.919	48.866		57.51	H
MOTA	2800	CB	TYR	152	152.646	27.131	50.342	1.00	55.56	H
ATOM	2801	CG '	TYR	152	152.211	28.529	50.695	1.00	49.75	H
MOTA	2802	CD1	TYR	152	150.893	28.938	50.497	1.00	37.14	H

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ATOM	2803	CE1	TYR	152		150.474	30.222	50.847	1.00	37.53	H
ATOM	2804	CD2	TYR	152		153.104	29.437	51.250	1.00	44.59	H
ATOM	2805	CE2	TYR	152		152.696	30.726	51.605	1.00	49.92	H
ATOM	2806	CZ	TYR	152		151.379	31.107	51.400	1.00	51.57	H
MOTA	2807	ОН	TYR	152		150.967	32.371	51.745	1.00	62.33	Н
MOTA	2808	C	TYR	152		151.874	27.358	47.965	1.00	48.01	H
MOTA	2809	0	TYR	152		151.962	28.386	47.291	1.00	28.34	H
ATOM	2810	N	PHE	153		150.810	26.567	47.947	1.00	50.83	H
ATOM	2811	CA	PHE	153		149.646	26.857	47.125	1.00	59.21	H
MOTA	2812	CB	PHE	153		150.003	26.728	45.646	1.00	64.09	H
ATOM	2,813	CG	PHE	153		148.926	27.214	44.725	1.00	66.51	H
ATOM	2814	CD1	PHE	153		148.786	28.571	44.464	1.00	66.83	H
ATOM	2815	CD2	PHE	153		148.036	26.323	44.147	1.00	60.06	H
ATOM	2816	CE1	PHE	153		147.770	29.037	43.638	1.00	55.52	H
MOTA	2817	CE2	PHE	153	•	147.013	26.775	43.316	1.00	50.07	H
MOTA	2818	CZ	PHE	153		146.880	28.138	43.061	1.00	49.86	H
ATOM	2819	C	PHE	153		148.499	25.907	47.449	1.00	52.00	H
ATOM	2820	0	PHE	153		148.709	24.702	47.619	1.00	57.40	H
ATOM	2821	N	PRO	154		147.265	26.436	47.538	1.00	46.46	H
ATOM	2822	CD	PRO	154		146.057	25.644	47.815	1.00	39.60	H
MOTA	2823	CA	PRO	154		146.931	27.851	47.353	1.00	44.22	H
ATOM	2824	CB	PRO	154		145.533	27.795	46.772	1.00	48.46	H
ATOM	2825	CG	PRO	154	,	144.923	26.614	47.482	1.00	49.48	H
ATOM	2826	С	PRO	154		146.932	28.559	48.694	1.00	48.75	H
ATOM	2827	. 0	PRO	154		147.255	27.958	49.722	1.00	45.97	H
MOTA	2828	\mathbf{N}	${ t GLU}$	155		146.573	29.835	48.683	1.00	45.51	H
MOTA	2829	CA	GLU	155		146.508	30.585	49.927	1.00	46.54	H
ATOM	2830,	CB	GLU	155	a	146.287	32.072	49.649	1.00	42.15	H
MOTA	2831	CG	GLU	155	2 for 1	147.565	32.888	49.519	1.00	52.55	H
MOTA	2832	CD	GLU	155		147.866	33.696	50.773	1.00	54.96	H
ATOM	2833	OE1	GLU	155		148.005	33.096	51.862	1.00	38.84	H
MOTA	2834	OE2	GLU	155		147.964	34.938	50.667	1.00	57.00	H
ATOM	2835	C	GLU	155		145.292	30.003	50.625	1.00	43.57	H
ATOM	2836	0	GLU	155		144.445	29.388	49.974	1.00	52.29	H
ATOM	2837	N	PRO	156	•	145.203	30.148	51.953	1.00	28.63	H
MOTA	2838	CD	PRO	156	ı	143.990	29.751	52.682	1.00	21.85	H
MOTA	2839	CA	PRO	156		146.134	30.804	52.873	1.00	32.78	H
ATOM	2840	CB	PRO	156		145.212	31.685	53.699	1.00	41.77	H
MOTA	2841	CG	PRO	156		143.896	30.824	53.775	1.00	10.50	H
MOTA	2842	C	PRO	156		146.879	29.797	53.776	1.00	40.11	H
MOTA	2843	0	PRO	156		146.757	28.583	53.613	1.00	30.70	H
ATOM	2844	N	VAL	157	,	147.641	30.333	54.722	1.00	47.16	H
MOTA	2845	CA	VAL	157		148.383	29.540	55.693	1.00	58.27	H
MOTA	2846	CB	VAL	157		149.898	29.452	55.362	1.00	52.20	H
ATOM	2847	CG1	VAL	157		150.106	28.797	54.011	1.00	56.74	H
MOTA	2848	CG2	VAL	157		150.525	30.837	55.387	1.00	45.36	H
MOTA	2849	C	VAL	157		148.239	30.258	57.032	1.00	68.19	H
MOTA	2850	0	VAL	157		147.993	31.466	57.076	1.00	78.90	H
MOTA	2851	N	THR	158		148.395	29.520	58.122	1.00	68.08	H
ATOM	2852	CA	THR	158		148.282	30.116	59.442	1.00	63.24	H
ATOM	2853	CB	THR	158		147.209	29.396	60.279	1.00	61.67	H
ATOM	2854	OG1	THR	158		145.962	29.426	59.573	1.00	52.99	H
MOTA	2855	CG2	THR	158		147.034	30.079	61.632	1.00	56.86	H

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ATOM	2856	C	THR	158	149.623	30.035	60.154	1.00	64.54		H
MOTA	2857	0	THR	158	150.187	28.954	60.312		65.02		\mathbf{H}
MOTA	2858	N	LAV	159	150.131	31.190	60.571		48.72	. ·	H
MOTA	2859	CA	VAL	159	151.409	31.266	61.256	1.00	38.04		H
MOTA	2860	CB	VAL	159	152.384	32.209	60.517	1.00	35.68	. :	H
MOTA	2861	CG1	VAL	159	153.745	32.207	61.195	1.00	13.69		H
MOTA	2862	CG2	VAL	159	152.520	31.765	59.072	1.00	35.33	ı	H
MOTA	2863	C	VAL	159	151.239	31.746	62.690	1.00	32.37	•	H
MOTA	2864	0	VAL	159	150.940	32.917	62.951	1.00	46.22		H
MOTA	2865	N	THR	160	151.430	30.812	63.616	1.00	34.81		H
MOTA	2866	CA	THR	160	151.316	31.088	65.037	1.00	30.02	,	H
MOTA	2867	CB	THR	160	150.305	30.146	65.702	1.00	29.19		H
ATOM	2868	OG1	THR	160	149.788	29.230	64.729	1.00	41.86		H
ATOM	2869	CG2	THR	160	149.165	30.943	66.295	1.00	40.64		H
ATOM	2870	C	THR	160	152.676	30.872	65.681	1.00	28.21		H
MOTA	2871	O	THR	160	153.501	30.118	65.169	1.00	44.55		H
ATOM	2872	N	TRP	161	152.909	31.546	66.800	1.00	43.52 54.28		H
ATOM	2873	CA	TRP	161	154.171	31.404	67.506 67.672		46.91		H
ATOM	2874	CB	TRP	161	154.833 155.369	32.773 33.327	66.379	1.00	31.10		H
MOTA	2875	CG	TRP	161	156.648	33.327	65.790		39.01		H
ATOM	2876 2877	CD2 CE2	TRP TRP	161 161	156.710	33.782	64.579	1.00	43.01		H
ATOM ATOM	2878	CE3	TRP	161	157.748	32.277	66.169	1.00	31.39		H
ATOM	2879	CD1	TRP	161	154.727	34.179	65.525		30.94		H
ATOM	2880	NE1	TRP	161	155.525	34.458	64.443		31.32	1	H
MOTA	2881	CZ2	TRP	161	157.829	33.749	63.741		35.89		H
MOTA	2882	CZ3	TRP	161	158.861	32.242	65.335		23.31		H
ATOM	2883	CH2	TRP	161	158.893	32:975	64.134		38.71		H
ATOM	2884	C	TRP	161	153.920	30.746	68.862		57.21		H
ATOM	2885	0	TRP	161	153.157	31.255	69.691	1.00	61.27		H
ATOM	2886	N	ASN	162	154.569	29.602	69.071	1.00	56.37		H
ATOM	2887	CA	ASN	162	154.426	28.829	70.298		50.72		H
ATOM	2888	CB	ASN	162	154.818	29.676	71.515	1.00	39.98		H
MOTA	2889	CG	ASN	162	156.331	29.771	71.698	1.00	45.87		H
ATOM	2890	OD1	ASN	162	157.103	29.298	70.854	1.00	61.54		H
ATOM	2891	ND2	ASN	162	156.760	30.385	72.801	1.00	49.15	,	H
ATOM	2892	C	ASN	162	152.979	28.365	70.399	1.00	44.59	ı	H
ATOM	2893	0	ASN	162	152.387	28.329	71.479	1.00	33.04	1	H
MOTA	2894	\mathbf{N}	SER	163	152.419	28.021	69.242	1.00	55.71		\mathbf{H}
MOTA	2895	CA	SER	163	151.048	27.541	69.133	1.00	65.28		H
ATOM	2896	CB	SER	163	150.858	26.313	70.021	1.00	69.26		\mathbf{H}
ATOM	2897	OG	SER	163	151.917	25.391	69.823	1.00	87.88		$\mathbf{H}^{'}$
MOTA	2898	C	SER	163	149.993	28.592	69.468	1.00	64.07		H
MOTA	2899	0	SER	163	148.799	28.363	69.267	1.00	71.86		H
ATOM	2900	N	GLY	164	150.430	29.744	69.970	1.00	56.72		H
MOTA	2901	CA	GLY	164	149.490	30.798	70.308	1.00	44.67	a .	H
ATOM	2902	C	GLY	164	149.953	31.629	71.482	1.00	45.89		H
ATOM	2903	0	GLY	164	149.611	32.807	71.597		41.13		H
MOTA	2904	N	SER	165	150.739	31.011	72.355		56.45		H
MOTA	2905	CA	SER	165	151.259	31.688	73.533		57.02		H
MOTA	2906	CB	SER	165	152.169	30.745	74.316		62.37		H
ATOM	2907	OG	SER	165	151.418	29.663	74.836		50.35		H
ATOM	2908	C	SER	165	152.020	32.945	73.153	1.00	57.97		H

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MOTA	2909	0	SER	165	152.276	33.809	73.989	1.00 41.07	H
MOTA	2910	N	LEU	166	152.385	33.049	71.883	1.00 64.03	H
MOTA	2911	CA	LEU	166	153.102	34.227	71.421	1.00 56.74	H
ATOM	2912	CB	LEU	166	154.493	33.841	70.923	1.00 37.44	H
MOTA	2913	CG	LEU	166	155.626	34.088	71.922	1.00 41.79	H
MOTA	2914	CD1	LEU	166	156.948	33.782	71.254	1.00 36.73	H
MOTA	2915	CD2	LEU	166	155.598	35.532	72.416	1.00 58.45	H
MOTA	2916	C	LEU	166	152.318	34.920	70.319	1.00 60.22	H
MOTA	2917	0	LEU	166	152.399	34.547	69.147	1.00 63.00	H
MOTA	2918	N	SER	167	151.547	35.928	70.708	1.00 65.96	H
MOTA	2919	CA	SER	167	150.740	36.684	69.762	1.00 64.77	H
ATOM	2920	CB	SER	167	149.255	36.347	69.946	1.00 66.65	H
MOTA	2921	OG	SER	167	148.697	37.030	71.057	1.00 54.23	H
MOTA	2922	C	SER	167	150.978	38.172	69.977	1.00 65.40	H
MOTA	2923	0	SER	167	150.141	39.009	69.637	1.00 63.94	H
MOTA	2924	N	SER	168	152.134	38.486	70.548	1.00 72.22	H
MOTA	2925	CA	SER	168	152.515	39.868	70.814	1.00 66.97	H
MOTA	2926	CB	SER	168	152.814	40.052	72.306	1.00 83.10	H
MOTA	2927	OG	SER	168	153.476	41.282	72.551	1.00 92.96	H
MOTA	2928	C	SER	168	153.754	40.212	69.997	1.00 58.05	H
ATOM	2929	0	SER	168	154.694	39.422	69.922	1.00 58.07	H
ATOM	2930	N	GLY	169	153.754	41.392	69.381	1.00 49.62	H
ATOM	2931	CA	GLY	169	154.897	41.799	68.582	1.00 43.99	\mathbf{H}
MOTA	2932	C	GLY	169	155.088	40.916	67.366	1.00 44.05	. H
MOTA	2933	0	GLY	169	156.205	40.731	66.887	1.00 49.35	H
MOTA	2934	N	VAL	170	153.991	40.366	66.862	1.00 45.75	H
MOTA	2935	CA	VAL	170	154.058	39.506	65.697	1.00 34.35	H
ATOM	2936	CB	VAL	170	153.135	38.291	65.854	1.00 29.09	H
ATOM	2937	CG1		170	153,213	37.418	64.614	1.00 23.76	H
ATOM .	2,938	CG2		170	153.539	37.492	67.079	1.00 30.40	H.
ATOM	2939	C	VAL	170	153.660	40.269	64.445	1.00 37.22	H
ATOM	2940	0	VAL	170	152.732	41.074	64.460	1.00 35.69	H
ATOM	2941	N	HIS	171	154.383	40.017	63.364	1.00 38.69	H
ATOM	2942	CA	HIS	171 .	154,118	40.664	62.088	1.00 33.69	H
ATOM	2943	CB	HIS	171	155.167	41.743	61.802	1.00 38.36	H
ATOM	2944	CG	HIS	171	155.011	42.971	62.636	1.00 40.32	H
ATOM	2945	CD2	HIS	171	155.806	44.055	62.783	1.00 49.35	H
ATOM	2946		HIS	171	153.923	43.182	63.456	1.00 58.85	H
ATOM	2947		HIS	171	154.053	44.343	64.068	1.00 58.33	H
MOTA	2948	NE2		171	155.189	44.896	63.678	1.00 51.33	H
ATOM	2949	C	HIS	171	154.172	39.623	60.985	1.00 37.90	H
ATOM	2950	0	HIS	171	155.251	39.144	60.626	1.00 52.25	H
ATOM	2951	N	THR	172	153.012	39.250	60.465	1.00 36.40	H
ATOM	2952	CA	THR	172	152.974	38.289	59.379	1.00 37.99	H
ATOM	2953	CB	THR	172	151.865	37.251	59.576	1.00 30.37	H
ATOM	2954	OG1	THR	172 ,	152.160	36.452	60.729		H
ATOM	2955	CG2		172	151.760	36.351	58.356	1.00 18.72	H
ATOM	2956	C	THR	172	152.708	39.097	58.118	1.00 43.29	H
MOTA	2957	O	THR	172	151.690	39.782	58.011	1.00 42.87	H
ATOM	2958	N	PHE	173	153.635	39.031	57.172	1.00 42.03	H
ATOM	2959	CA	PHE	173	153.500	39.783	55.935	1.00 41.59	H
ATOM	2960	CB	PHE	173	154.889	40.102	55.372	1.00 69.43	H
MOTA	2961	CG	PHE	173	155.707	40.945	56.285	1.00 69.16	H

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MOTA	2962	CD1	PHE	173	155.577	42.326	56.264	1.00 69.14	· H
MOTA	2963	CD2	PHE	173	156.555	40.360	57.216	1.00 71.48	H
ATOM	2964	CE1	PHE	173	156.277	43.117	57.165	1.00 47.16	H
ATOM	2965	CE2	PHE	173	157.260	41.140	58.122	1.00 46.77	H
ATOM	2966	CZ.	PHE	173	157.120	42.523	58.097	1.00 50.06	H
ATOM	2967	C	PHE	173	152.651	39.103	54.870	1.00 51.94	H
MOTA	2968	0	PHE	173	152.670	37.881	54.715	1.00 45.37	H
ATOM	2969	N	·PRO .	174	151.873	39.901	54.128	1.00 47.56	H
MOTA	2970	CD	PRO	174	151.760	41.360	54.268	1.00 40.08	H
MOTA	2971	CA	PRO	174	151.010	39.369	53.070	1.00 39.95	H
ATOM	2972	CB	PRO	174	150.417	40.618	52.419	1.00 38.02	H
ATOM	2973	CG	PRO	174	151.234	41.778	52.945	1.00 41.70	H
MOTA	2974	C	PRO	174	151.793	38.515	52.080	1.00 34.30	H
MOTA	2975	0	PRO	174	152.926	38.844	51.719	1.00 38.61	H
MOTA	2976	N	ALA	175	151.191	37.407	51.655	1.00 33.98	H
MOTA	2977	. CA	ALA	175	151.834	36.505	50.711	1.00 28.24	H
ATOM	2978	CB	ALA	175	150.947	35.303	50.455	1.00 24.04	H
MOTA	2979	C	ALA	175	152.106	37.226	49.411	1.00 43.10	H
ATOM	2980	0	ALA	175	151.420	38.182	49.064	1.00 41.83	H
ATOM	2981	N	VAL	176	153.119	36.758	48.691	1.00 47.34	H
MOTA	2982	CA	VAL	176	153.479	37.340	47.409	1.00 46.04	H
MOTA	2983	CB	VAL	176	154.660	38.335	47.546	1.00 48.76	H
ATOM	2984	CG1		176	155.822	37.686	48.280	1.00 50.38	H
ATOM	2985	CG2	VAL	176	155.100	38.809	46.167	1.00 64.07	H
MOTA	2986	C	VAL	176	153.858	36.205	46.462	1.00 36.12	H
ATOM	2987	0	VAL	176	154.544	35.263	46.857	1.00 30.73	H
MOTA	2988	N	LEU	177	153.392	36.298	45.220	1.00 48.02	H
ATOM	2989	CA	LEU 	177	153.647	35.282	44.205	1.00 60.32	H
ATOM	2990	CB	LEU	177	152.686	35.467	43,036	1.00 39.51	H
ATOM	2991	CG	LEU	177	152.048	34.165		1.00 27.99	H
ATOM	2992	CD1		177	151.014	33.698	43.572	1.00 30.57	H
ATOM	2993	CD2	LEU	177	151.410	34.378	41.197	1.00 38.71	H
ATOM	2994	C	LEU	177	155.074	35.257	43.679	1.00 73.61	H H
ATOM	2995	0	LEU	177	155.621	36.275	43.254	1.00 78.42	Н
ATOM	2996	N	GLN	178	155.669	34.074 33.895	43.694 43.227	1.00 79.08 1.00 95.82	Н
ATOM	2997	CA	GLN	178	157.031	33.932	44.432	1.00 95.82	H
ATOM	2998	CB	GLN	178 178	157.981 · 159.244	33.932	44.308	1.00 99.99	H
ATOM	2999	CG CD	GLN GLN	178	160.357	33.583	45.224	1.00 99.99	H
ATOM	3000 3001	OE1	GLN	178	160.327	33.367	46.439	1.00 98.52	H
ATOM ATOM	3001	NE2	GLN	178	161.350	34.244	44.637	1.00 99.99	H
ATOM	3002	C	GLN	178	157.123		42.483	1.00 99.99	H
ATOM	3003	0	GLN	178	157.289	31.504	43.092	1.00 99.97	H
ATOM	3004	N	SER	179	156.984	32.637	41.159	1.00 96.75	H
ATOM	3005	CA	SER	179	157.047	31.465	40.289	1.00 87.63	H
ATOM	3007	CB	SER	179	158.307	30.641	40.589	1.00 93.06	H
ATOM	3007	OG	SER	179	159.098	30.472	39.425	1.00 67.71	H
ATOM	3009	C	SER	179	155.815	30.580	40.430	1.00 81.94	H
ATOM	3010	0	SER	179	155.927	29.351	40.461	1.00 85.05	H
ATOM	3010	N	ASP	180	154.649	31.217	40.517	1.00 61.79	H
ATOM	3011	CA	ASP	180	153.367	30.518	40.643	1.00 53.42	H
ATOM	3012	CB	ASP	180	153.284	29.372	39.633	1.00 63.39	H
ATOM	3013	CG	ASP	180	152.902	29.846	38.251	1.00 90.41	H
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MOTA	3015	OD1	ASP	180	ī	151.736	30.262	38.066	1.00	95.28	·H
ATOM	3016	OD2	ASP	180	*	153.771	29.804	37.350	1.00	91.35	H
ATOM	3017	C	ASP	180		153.036	29.975	42.030	1.00	48.83	H
MOTA	3018	0	ASP	180		151.965	29.414	42.234	1.00	32.55	H
MOTA	3019	N	LEU	181	•	153.955	30.120	42.976	1.00	49.73	H
MOTA	3020	CA	LEU	181		153.716	29.646	44.332	1.00	42.63	H
MOTA	3021	CB	LEU	181		154.751	28.594	44.730	1.00	51.61	H
MOTA	3022	- CG	LEU	181		154.817	27.335	43.865	1.00	45.19	H
MOTA	3023	CD1	LEU	181		155.788	26.358	44.503	1.00	36.88	H
MOTA	3024	CD2	LEU	181		153.429	26.712	43.723	1.00	49.90	H
MOTA	3025	C	LEU	181		153.811	30.840	45.265	1.00	36.09	H
MOTA	3026	0	· LEU	181,	•	154.401	31.859	44.914	1.00	47.48	. H
MOTA	3027	N	TYR	182		153.235	30.711	46.454	1.00	34.48	H
MOTA	3028	CA	TYR	182		153.254	31.803	47.410	1.00	34.99	H
ATOM	3029	CB	TYR	182		151.965	31.824	48.221	1.00	43.15	H
MOTA	3030	CG	TYR	182		150.768	32.266	47.431	1.00	26.23	H
MOTA	3031	CD1	TYR	182		150.514	33.621	47.219	1.00	24.46	H
MOTA	3032	CE1	TYR	182		149.437	34.034	46.455	1.00	26.76	H
MOTA	3033	CD2	TYR	_. 182		149.908	31.332	46.864	1.00	28.50	H
MOTA	3034	CE2	TYR	182	10	148.827	31.733	46.097	1.00		\mathbf{H}_{s}
MOTA	3035	CZ	TYR	182		148.596	33.085	45.893	1.00	31.63	H
MOTA	3036	OH	TYR	182		147.538	33.480	45.108	1.00	52.38	H
MOTA	3037	. C	TYR	182		154.410	31.694	48.361	1.00	34.67	H
MOTA	3038	0	TYR	182		154.902	30.604	48.642	1.00		H
ATOM	3039	N	THR	183		154.842	32.844	48.860	1.00	46.64	H
ATOM	3040	CA	THR	183		155.915	32.914	49.838	1.00	32.69	H
ATOM	3041	CB	THR	183		157.250	33.348	49.232	1.00	32.26	H
ATOM	3042	OG1		183		157.678	32.396	48.250	1.00	39.58	H
MOTA	3043	CG2		183		158.288	33.442	50.318	1.00	33.99	. H
ATOM	3044	C,	THR	183		155.483	33.981	50.823	1.00	28.00	H
ATOM	3045	0	THR	183	1	154.927	35.009	50.440	1.00	38.20	H
ATOM	3046	N	LEU	184		155.737	33,743	52.097	1.00	27.54	H
ATOM	3047	CA	LEU	184		155.353	34.696	53.114	1.00	30.19	H
MOTA	3048	CB	LEU	184		153.926	34.380	53.559	1.00	30.95	H
MOTA	3049	CG	LEU	184		153.483	34.617	54.996	1.00	46.42	H
ATOM	3050	CD1	LEU	184		151.969	34.814	55.016	1.00	25.32	H
ATOM	3051	CD2	LEU	184		153.891	33.439	55.867		45.00	H
ATOM	3052	C	LEU	184		156.337	34.598	54.271	*	30.88	H
ATOM	3053	0	LEU	184		157.075	33.623	54.383		17.03	H
ATOM	3054	N	SER	185		156.370	35.613	55.122		29.51	H
ATOM	3055	CA	SER	185		157.278	35.599		1.00		H
ATOM	3056	CB	SER	185		158.573	36.350	55.914		21.45	H
MOTA	3057	OG G	SER	185		158.354	37.749	55.844		46.01	H
MOTA	3058	C	SER	185		156.610	36.235	57.449		28.20	H
MOTA	3059	0	SER	185		155.828	37.173	57.312		26.88	H
MOTA	3060	N	SER	186		156.917	35.710	58.625		38.58	H
ATOM	3061	CA	SER	186		156.354	36.229	59.853		34.31	H
ATOM	3062	CB	SER	186 186		155.389	35.210	60.463	1.00	37.09	H
MOTA	3063	OG G	SER	186 186		154.862	35.685	61.689		44.43	H
ATOM	3064	C	SER	186		157.487	36.510	60.822			H
ATOM	3065	0	SER	186	-	158.356	35.663	61.036	1.00	38.29	H
ATOM	3066	N	SER	187		157.491	37.703	61.395		15.70	H
MOTA	3067	CA	SER	187		158.524	38.066	62.348	T.00	25.23	H

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MOTA	3068	CB	SER	187	,	159.100	39.440	62.008	1.00	18.98		H
ATOM	3069	OG	SER	187		158.187	40.466	62.346	1.00	36.58		Ħ
ATOM	3070	C	SER	187		157.905	38.092	63.739	1.00	27.63		\cdot H
ATOM	3071	Ο .	SER	187		156.692	38.240	63.882	1.00	26.02		H
ATOM	3072	N	VAL	188 -		158.739	37.926	64.762.	1.00	31.12		H
ATOM	3073	CA	VAL	188	i	158.266	37.950	66.141	1.00	31.94		\mathbf{H}
MOTA	3074	CB	VAL	188		157.996	36.524	66.681	1.00	32.97		H
MOTA	3075	CG1	VAL	188	•	159.298	35.776	66.878	1.00	21.32		H
MOTA	3076	CG2	VAL	188		157.221	36.606	67.987	1.00	48.09		\mathbf{H}
MOTA	3077	C ·	VAL	188		159.284	38.646	67.030	1.00	29.00		H
MOTA	3078	0	VAL	188		160.469	38.322	67.016	1.00	18.81		H
MOTA	3079	\mathbf{M}^{\cdot}	THR	189		158.811	39.618	67.799	1.00	43.09		H
MOTA	3080	CA	THR	189		159.664	40.385	68.691	1.00	52.62		H
MOTA	3081	CB	THR	189	,	159.381	41.890	68.535	1.00	55.64		H
ATOM	3082	OG1	THR	189		159.915	42.346	67.288	1.00	72.06		H
ATOM	3083	CG2	THR	189		160.006	42.678	69.676	1.00	47.82		H
ATOM	3084	C	THR	189		159.450	39.981	70.147	1.00	47.05		H
ATOM	3085	0	THR	189		158.313	39.914	70.622	1.00	51.99	•	H
ATOM	3086	N	VAL	190		160.547	39.715	70.846	1.00	33.42		H
ATOM	3087	CA	VAL	190		160.489	39.327	72.251	1.00	49.20		H
MOTA	3088	CB	VAL	190		160.501	37.795	72.408	1.00	46.79		H
MOTA	3089	CG1	VAL	190		159.222	37.205	71.839	1.00	24.58		H
MOTA	3090	CG2	VAL	190	4	161.717	37.217	71.715	1.00	27.47		H
MOTA	3091	C	VAL	190	•	161.670	39.893	73.037	1.00	57.65		$_{\cdot}$ H
MOTA	3092	0	VAL	190		162.797	39.935	72.538	1.00	35.32		H
MOTA	3093	N	PRO	191		161.419	40.347	74.277	1.00	74.09		H
MOTA	3094	CD	PRO	191		160.096	40.363	74.931	1.00	85.05		H
MOTA	3095	CA	PRO	191		162.461	40.912	75.142	1.00	73.28		H
MOTA	3096	CB	PRO	191	٠	161.769	41.033	76.496	1.00	85.43		H
ATOM	3097	CG	PRO	191		160.328	41.206	76.155	1.00	90.65		H
ATOM	3098	C	PRO	191 .		163.708	40.031	75.207	1.00	69.24		H
ATOM	3099	0	PRO	191		163.618	38.814	75.392	1.00	45.94		H
MOTA	3100	N	SER	192		164.871	40.663	75.063	1.00	75.06		H
MOTA	3101	CA.	SER	192		166.146	39.952	75.082	1.00	71.45		H
MOTA	3102	CB	SER	192		167.311	40.955	75.103	1.00	59.57		H
MOTA	3103	OG	SER	192		167.154	41.923	76.129	1.00	83.36		H
MOTA	3104	C	SER	192	•	166.291	38.977	76.248	1.00	74.48		H
MOTA	3105	0	SER	192		167.095	38.051	76.184	1.00	78.55		H
ATOM	3106	\boldsymbol{N}	SER	193	4	165.498	39.169	77.297	1.00	78.60		H
MOTA	3107	CA	SER	193		165.574	38:315	78.476	1.00	75.62		H
MOTA	3108	CB	SER	193		164.901	39.019	79.661	1.00	88.02		H
MOTA	3109	OG	SER	193	*	163.490	39.027	79.525	1.00	99.66		H
ATOM	3110	C	SER	193		165.013	36.898	78.345	1.00	67.52		H
ATOM	3111	0	SER	193		165.430	35.998	79.073	1.00	55.75		H
MOTA	3112	\boldsymbol{N}	THR	194		164.083	36.684	77.418	1.00	72.49		H
ATOM	3113	CA	THR	194		163.464	35.365	77.259	1.00	71.00		H
ATOM	3114	CB	THR	194		161.967	35.507	76.936		85.22		H
ATOM	3115	OG1	THR	194	4	161.795	36.425	75.846	1.00	87.88		H
ATOM	3116	CG2	THR.	194		161.213	36.023	78.15,4	1.00	86.98	•	H
ATOM	3117	C	THR	194		164.082	34.432	76.219	1.00	51.89		H
ATOM	3118	0 .	THR	194		163.726	33.253	76.150	1.00	40.90		H
MOTA	3119	N	TRP	195		164.996	34.957	75.408	1.00	50.33		H
ATOM	3120	CA	TRP	195		165.654	34.154	74.381	1.00	48.60	ı	H

MOTA	3121	CB TRP	195	165.109	34.515 72.9	90 1.00 43.1	2 H
MOTA	3122	CG TRP	195	165.338	33.444 71.9	45 1.00 ₀ 50.9	2 . H
MOTA	3123	CD2 TRP	195	166.332	33.451 70.9	07 1.00 56.4	8 H
ATOM	3124	CE2 TRP	195	166.199	32.235 70.1	92 1.00 47.6	б н
MOTA	3125	CE3 TRP	195	167.320	34.365 70.5	13 1.00 53.3	
MOTA	3126	CD1 TRP	195	164.664	32.259 71.8		
MOTA	3127	NE1 TRP	195	165.175	31.528 70.7		
ATOM	3128	CZ2 TRP	195	167.019	31.911 69.1		·
MOTA	3129	CZ3 TRP	195	168.136	34.040 69.4		
ATOM	3130	CH2 TRP	195	167.979	32.821 68.7		
MOTA	3131	C TRP	195	167.164	34.383 74.4		
MOTA	3132	O TRP	195	167.620	35.492 74.7		
MOTA	3133	N PRO	196	167.960	33.334 74.1		
ATOM	3134	CD PRO	196	169.426	33.449 74.1		
MOTA	3135	CA PRO	.196	167.526	31.972 73.8		
ATOM	3136	CB PRO	196	168.764	31.339 73.1		
ATOM	3137	CG PRO	196	169.812	32.444 73.0		
ATOM	3138	C PRO	196	167.047	31.179 75.0		
ATOM	3139	O PRO	196	166.920	29.951 74.9		
ATOM	3140	N SER	197	166.789	31.891 76.1		
ATOM	3141	CA SER	197	166.315	31.282 77.3		
ATOM	3142	CB SER	197	165.718	32.353 78.2 32.329 79.5		
MOTA	3143	OG SER	197	166.324	32.329 79.5 30.225 77.0		
MOTA	3144	C SER	197	165.261	29.029 76.9		•
MOTA	3145	O SER	197	165.557 164.032	30.680 76.8		•
MOTA	3146 3147	N GLU CA GLU	198 198	162.925	29.787 76.4		
ATOM ATOM	3148	CA GLU	198	161.605	30.416 76.9		
ATOM	3149	CG GLU	198	161.645	30.972 78.3		
ATOM	3150	CD GLU	198	160.646	32.093 78.5		
ATOM	3151	OE1 GLU	198	159.817	32.341 77.6		•
ATOM	3152	OE2 GLU	198	160.689	32.725 79.6		
ATOM	3153	C GLU	198	162.889	29.516 74.9		
ATOM	3154	O GLU	198	163.247	30.384 74.2		
ATOM	3155	N THR	199	162.462	28.314 74.6	14 1.00 54.93	3 н
ATOM	3156	CA THR	199	162.392	27.937 73.2	03 1.00 53.5	1 H
ATOM	3157	CB THR	199	162.304	26.400 73.0	31 1.00 61.1	8 H
MOTA	: 3158	OG1 THR	199	161.128	25.903 73.6	81 1.00 51.2	5 H
MOTA	3159	CG2 THR	199	163.536	25.727 73.6	23 1.00 78.0	7 H
ATOM ·	3160	C THR	199	161.205	28.583 72.4	85 1.00 59.63	3 H
MOTA	3161	O THR	199	160.120	28.730 73.0	54 1.00 59.9	8 H
ATOM	3162	N VAL	200	161.429	28.966 71.2	28 1.00 57.2	5 H
MOTA	3163	CA VAL	200	160.407	29.603 70.4	05 1.00 51.9	б н
MOTA	3164	CB VAL	200	160.815	31.039 70.0	35 1.00 33.42	2 H
MOTA	3165	CG1 VAL	200	159.951	31.540 68.8	99 1.00 17.7	5 H
MOTA	3166	CG2 VAL	200	160.680	31.944 71.2	39 1.00 31.9	
ATOM .	3167	C VAL	200	160.195	28.832 69.1	12 1.00 51.6	
MOTA	3168	O VAL	200	161.136	28.613 68.3		
MOTA	3169	N THR	201	158.955	28.427 68.8		
MOTA	3170	CA THR	201	158.631	27.684 67.6		
ATOM	3171	CB THR	201	158.116	26.267 67.9		
ATOM	3172	OG1 THR	201	159.042	25.602 68.8	**	
MOTA	3173	CG2 THR	201	157.949	25.458 66.6	88 1.00 39.8	7 H

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MOTA	3174	a C	THR	201	:	157.545	28.399	66.860	1.00	26.58	H
MOTA	3175	0	THR	201	,	156.682	29.055	67.438	1.00	25.18	H
ATOM	3176	N	CYS	202		157.593	28.279	65.538	1.00	22.39	\mathbf{H}
ATOM	3177	CA	CYS	202		156.582	28.902	64.699	1.00	25.43	H
ATOM	3178	,C	CYS	202		155.765	27.777	64.064	1.00	25.96	H
ATOM	3179	0	CYS	202		156.324	26.826	63.522	1.00		Н
ATOM	3180	· CB	CYS	202		157.243	29.820	63.649	1.00		· H
ATOM	3181	SG	CYS.	202		157.564	29.150	61.983	1.00		H
ATOM	3182	N	ASN	203		154.441	27.871	64.172		24.52	H
ATOM	3183	CA	ASN	203		153.554	26.842	63.628		29.46	Н
ATOM	3184	CB	ASN	203		152.539	26.387	64.686		36.69	Н
ATOM	3185	CG	ASN	203		152.926	26.807	66.099	1.00		H
ATOM	3186	OD1		203		152.586	27.904	66.552	1.00		H
ATOM	3187	ND2		203		153.629	25.926	66.805	1.00	33.32	H
ATOM	3188	C	ASN	203		152.800	27.293	62.389	1.00	18.74	Н
ATOM	3189	0	ASN	203		151.964	28.196	62.447	1.00	38.03	Н
ATOM	3190	N	VAL	204		153.099	26.646	61.270	1.00	23.45	H
ATOM	3191	CA	VAL	204		152.451	26.957	60.006	1.00	38.87	Н
ATOM	3192	CB	VAL	204		153.473	27.049	58.853	1.00	39.50	H
ATOM	3193	CG1	VAL	204		152.795	27.575	57.599	1.00	52.52	$^{-}$ ${f H}$
ATOM	3194	CG2		204		154.624	27.944	59.254	1.00	29.99	H
ATOM	3195	C ·	VAL	204		151.461	25.854	59.676	1.00	41.89	H
ATOM	3196	0	VAL	204		151.733	24.682	59.919	1.00	46.77	H
ATOM	3197	N	ALA	205	£	150.312	26.236	59.126	1.00	41.52	H
ATOM	3198	CA	ALA	205		149.285	25.273	58.751	1.00	32.14	H
ATOM	3199	CB	ALA	205		148.156	25.281	59.777	1.00	44.74	H
MOTA	3200	C	ALA	205		148.749	25.614	57.365	1.00	28.16	H
ATOM	3201	0	ALA	205		148.349	26.750	57.104	1.00	23.06	${\tt H}$
ATOM	3202	$oldsymbol{N}$.	HIS	206		148.756	24.629	56.474	1.00	38.89	H
ATOM	3203	CA	HIS	206		148.267	24.825	55.121	1.00	.31.01	H
ATOM	3204	CB	HIS	206		149.357	24.497	54.112	1.00	34.08	H
ATOM	3205	CG	HIS	206		149.025	24.909	52.715	1.00	25.51	H
ATOM	3206	CD2	HIS	206		148.521	26.065	52.227	1.00	33.37	H
MOTA	3207	ND1	HIS'	206		149.193	24.073	51.635	1.00	28.36	H
ATOM	3208	CE1	HIS	206		148.807	24.698	50.535	1.00	30.36	H
ATOM	3209	NE2	HIS	206		148.393	25.907	50.868	1.00	29.53	H
MOTA	3210	C	HIS	206		147.061	23.930	54.876	1.00	38.48	H
ATOM	3211	0	HIS	206	a	147.198	22.819	54.371	1.00	42.18	H
MOTA	3212	N	PRO	207		145.856	24.417	55.228	1.00	46.11	H
MOTA	3213	CD	PRO	207		145.636	25.758	55.802	1.00	59.24	H
MOTA	3214	CA	PRO	207		144.597	23.684	55.065	1.00	49.09	H
MOTA	3215	CB	PRO	207	,	143.538	24.780	55.138	1.00	55.68	H
MOTA	3216	CG	PRO	207		144.146	25.814	,56.018	1.00	65.42	H
MOTA	3217	G .	PRO	207	·	144.504	22.890	53.769	1.00	60.16	H
MOTA	3218	0	PRO	207		144.293	21.680	53.787	1.00	51.48	H
MOTA	3219	N	ALA	208		144.664	23.577	52.646	1.00	56.11	H
MOTA	3220	CA	ALA	208		144.584	22.933	51.342	1.00	41.51	H
MOTA	3221	CB	ALA	. 208		145.043	23.899	50.261		34.52	H
MOTA	3222	C	ALA	208		145.397	21.638	51.269		43.41	H
MOTA	3223	0	ALA	208		144.983	20.676	50.615		51.37	H
MOTA	3224	N	SER	209		146.550	21.615	51.933		47.62	H
MOTA	3225	CA	SER	209		147.396	20.424	51.923		48.72	H
ATOM	3226	CB	SER	209		148.852	20.811	51.634	1.00	44.67	H

			<i>?</i>	•		•	$x_{i_1} = x_{i_2}$		
ATOM	3227	OG	SER	209	149.387	21.642	52.650	1.00 55.80	H
ATOM	3228	C	SER	209	147.304	19.643	53.236	1.00 53.29	H
ATOM	3229	0	SER	209	147.973	18.624	53.411	1.00 52.35	H
ATOM	3230	N	SER	210.	146.462	20.119	54.148	1.00 71.17	H
ATOM	3231	CA	SER	210	146.269	19.475	55.444	1.00 82.90	H
ATOM	3232	CB	SER	210	145.509	18.158	55.277	1.00 90.95	H
ATOM	3233	OG	SER	210	144.137	18.333	55.578	1.00100.00	H
ATOM	3234	Ċ	SER	210	147.579	19.213	56.169	1.00 79.59	H
ATOM	3235	0	SER	210	147.702	18.234	56.908	1.00 80.94	H
ATOM	3236	N	THR	211	148.555	20.088	55.950	1.00 73.59	H
ATOM	3237	.CA	THR	211	149.854	19.964	56.594	1.00 75.14	${\tt H}$
ATOM	3238	CB	THR	211	151.027	20.111	55.599	1.00 76.28	H·
ATOM	3239	OG1	THR	211	150.990	21.414	55.008	1.00 73.09	H
ATOM	3240	CG2	THR	211	150.950	19.062	54.510	1.00 89.67	H
ATOM	3241	C	THR	211	150.024	21.051	57.643	1.00 74.45	H
ATOM	3242	0	THR	211	149.536	22.172	57.491	1.00 76.65	H
ATOM	3243	N	LYS	212	150.711	20.699	58.722	1.00 69.16	H
ATOM	3244	CA	LYS	212	150.988	21.645	59.783	1.00 61.67	H
ATOM	3245	CB	LYS	212	150.041	21.450	60.967	1.00 73.38	Н
ATOM	3246	CG	LYS	212	150.718	21.612	62.317	1.00 89.85	. Н
ATOM	3247	CD	LYS	212	150.006	22.614	63.192	1.00 99.99	H
ATOM	3248	CE	LYS	212	150.452	22.449	64.637	1.00 97.52	H
ATOM	3249	NZ	LYS	212	150.308	23.707	65.419	1.00 95.76	H
ATOM	3250	C	LYS	212	152.413	21.344	60.198	1.00 51.18	H
ATOM	3251	0	LYS	212	152.730	20.222	60.594	1.00 46.57	H
MOTA	3252	N	VAL	213	153.275	22.349	60.081	1.00 47.52	H
MOTA	3253	CA	VAL	213	154,672	22.201	60.434	1.00 33.06	H
ATOM	3254	CB	VAL	213	155.593	22.651	59.282	1.00 35.68	H
ATOM	3255	CG1	VAL	213	157.002	22.136	59.511	1.00 51.97	H
ATOM	3256	CG2	VAL	213	155.047	22.154	57.948	1.00 53.21	H
ATOM	3257	C ·	VAL	213	155.011	23.028	61.661	1.00 30.06	H
ATOM	3258	0.	VAL	213	154.324	23.996	61.991	1.00 34.34	H
ATOM	3259	N	ASP	214	156.071	22.625	62.343	1.00 35.26	Н
ATOM	3260	CA		214	156.541	23.325	. 63.523.	1.00 39.19	H
ATOM	3261	CB	ASP	214	156.228	22.526	64.791	1.00 58.41	H
MOTA	3262	CG	ASP	214	154.791	22.709	65.259	1.00 63.54	Н
ATOM	3263	OD1	ASP	214	154.397	23.857	65.553	1.00 65.10	H
ATOM	3264	OD2	ASP	214	154.059	21.699	65.336	1.00 80.45	H
ATOM	3265	C	ASP	214	158.046	23.454	63.342	1.00 37.64	H
ATOM	3266	0	ASP	214	158.725	22.489	62.983	1.00 41.00	H
ATOM	3267	N	LYS	215	158.564	24.652	63.564	1.00 34.85	H
ATOM	3268	CA	LYS	215	159.985	24.877	63.410	1.00 35.83	H
MOTA	3269	CB ;	LYS	215	160.261	25.637	62.112	1.00 37.75	H
ATOM	3270	CG	LYS	215	161.248	24.948	61.191	1.00 59.89	H
ATOM	3271	CD	LYS	215	160.536	23.992	60.251	1.00 59.31	H
MOTA	3272	CE	LYS	215	161.386	22.766	59.964	1.00 53.98	H
ATOM	3273	NZ	LYS	215	160.573	21.613	59.475	1.00 65.45	H
ATOM	3274	C	LYS	215	160.515	25.659	64.588	1.00 38.73	H
ATOM	3275	0	LYS	215	160.030	26.745	64.904	1.00 53.68	H
ATOM	3276	N	LYS	216	161.511	25.084	65.244	1.00 48.31	H
ATOM	3277	CA	LYS	216	162.141	25.714	66.389	1.00 47.35	H
ATOM	3278	CB	LYS	216	162.649	24.641	67.357	1.00 48.55	H
ATOM	3279	·CG	LYS	216	162.043	23.256	67.119	1.00 74.84	H
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MOTA	3280	CD	LYS	216	-	162.861	22.156	67.793	1.00	85.40	,	H
MOTA	3281	CE	LYS	216		162.592	22.085	69.296	1.00	94.97	•	H
MOTA	3282	NZ	LYS	216		162.133	20.733	69.738	1.00	92.19		H
ATOM	3283	C	LYS	216	>	163.305	26.543	65.860	1.00	46.24	•	H
MOTA	3284	0	LYS	216		163.898	26.203	64.838	1.00	34.41	•	H
ATOM	3285	N	ILE	217		163.622	27.637	66.541	1.00	41.02		H
ATOM	3286	CA	ILE	217		164.719	28.497	66.116	1.00	44.97		H
ATOM	3287	CB	ILE	217		164.273	29.978	66.046	1.00	41.86	:	H
MOTA	3288	CG2	ILE	217		165.094	30.716	64.991	1.00	44.48		H
ATOM	3289	CG1	ILE	217		162.768	30.063	65.749	1.00	33.66		H
ATOM	3290	CD1	ILE	217		162.407	30.038	64.270	1.00	17.95		H
ATOM	3291	C	ILE	217		165.890	28.363	67.094	1.00	47.47		H
MOTA	3292	0	ILE	217		165.690	28.400	68.310	1.00	43.27		H
MOTA	3293	N	VAL	218		167.103	28.219	66.559	1.00	50.40		H
ATOM	3294	CA	VAL	218		168.301	28.054	67.394	1.00	50.95		H
MOTA	3295	CB	VAL	218		169.003	26.705	67.084	1.00	57.08		H
ATOM	3296	CG1	VAL	218		167.974	25.686	66.599	1.00	55.44		H
MOTA	3297	CG2		218		170.105	26.903	66.037	1.00	73.39		H
MOTA	3298	C	VAL	218	ı	169.344	29.175	67.289	1.00	41.93		H
ATOM	3299	0	VAL	218		170.001	29.458	68.317	1.00			H
ATOM	3300	OT	VAL	218		170.011	29.390	69.119	1.00	52.14		H
ATOM	3301	CB	LYS	2		95.854	32.588	47.685	1:00	42.79		C
ATOM -	3302	CG	LYS	2		95.825	31.435	46.699	1.00	53.80		C
ATOM	3303	CD	LYS	2	*	94.407	30.925	46.486	1.00	62.43		C
ATOM	3304	CE	LYS	2		94.373	29.740	45.531	1.00	62.95	•	C
ATOM	3305	NZ	LYS	2		94.065	28.460	46.232	1.00	60.28	•	C
MOTA	3306	C	LYS	2		94.693	33.099	49.840	1.00	46.91		C
ATOM	3307	0	LYS	2	ı	93.606	32.673	50.239	1.00	58.66		C
MOTA	3308	N	LYS	2		95.259	30.740	49.234	1.00	34.71		C
ATOM	3309	CA	LYS	. 2		95.690	32.169	49.150	1.00	47.34		C
MOTA	3310	N	ILE	. 3		95.072	34.368	49.975	1.00	39.77		C
MOTA	3311	CA	ILE	. 3		94.226	35.372	50.621	1.00	41.61		C
ATOM	3312	CB	ILE	3 .		95.062	36.456	51.331	1.00	43.12	,	C
ATOM	3313	CG2	ILE	3		94.142	37.421	52.074	1.00	41.52		C
ATOM	3314	CG1	ILE	3 '	**	96.056	35.818	52.301	1.00	48.11		C
MOTA	3315	CD1	ILE	3		97.282	36.672	52.556	1.00	29.73		C
ATOM	3316	C	ILE	3		93.346	36.101	49.623	1.00	38.09		C
ATOM	3317	0	ILE	3		93.645	36.147	48.437	1.00	41.06		C
ATOM	3318	N	LEU	4		92.266	36.686	50.124	1.00	41.63		C
MOTA	3319	CA	LEU	4		91.349	37.439	49.287	1.00	47.21		C
ATOM	3320	CB	LEU	4	ı		37.026	49.581	1.00	47.90	-	C
ATOM	3321	CG	LEU	4		89.389	35.782	48.852	1.00	49.25	a	C
ATOM	3322	CD1	LEU	4		89.552	35.970	47.351	1.00	37.24		C
ATOM	3323	CD2	LEU	4		90.138	34.543	49.324	1.00	54.80		C
ATOM	3324	C	LEU	4		91.536	38.927	49.569		48.08		C
ATOM	3325	0	LEU	4		91.868	39.322	50.695		31.46		C
ATOM	3326	N	VAL	5		91.326	39.743	48.538		43.17		C
ATOM	3327	CA	VAL	, 5		91.469	41.190	48.660		33.62		C
ATOM	3328	CB	VAL	5		92.806	41.673	48.047		32.71		C
ATOM	3329	CG1	VAL	5		93.315	42.880	48.803		22.52		C
ATOM	3330	CG2	LAV	5 .		93.836	40.559	48.081		29.21		C
ATOM	3331	C	VAL	5		90.325	41.911	47.945		36.98		C
ATOM	3332	0	VAL	5		90.028	41.628	46.788		50.54		C
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ATOM	3333	N	LYS	,	6	,	89.689	42.844	48.640	1.00	39.70		C .
MOTA	3334	CA	LYS		6		88.593	43.622	48.068	1.00	41.54		C
MOTA	3335	CB	LYS		б	*	87.299	43.378	48.857	1.00	38.28		C
MOTA	3336	CG	LYS		б		86.443	42.233	48.341	1.00	48.43	•	C
MOTA	3337	CD	LYS		6		85.343	41.841	49.339	1.00	58.62		C
MOTA	3338	CE	LYS		, б		85.905	41.158	50.593	1.00	47.34		C
MOTA	3339	NZ	LYS	**	б		86.645		50.281	1.00	51.47		C
MOTA	3340	C	LYS		6		88.957	45.108	48.147	1.00	32.95		C
MOTA	3341	0	LYS		6	*	89.265	45.614	49.222	1.00	43.88		C
MOTA	3342	N	GLN		7		88.926	45.805	47.021	1.00	30.15		C
ATOM	3343	CA	GLN		7		89.258	47.224	47.022	1.00			C
ATOM	3344	CB	GLN		7		90.631	47.449	46.395	1.00			C
ATOM	3345	CG	GLN		7		91.355	46.178	46.002	1.00	48.85		C
MOTA	3346	CD	GLN		7		92.745	46.462	45.467	1.00	53.95		C
ATOM	3347	OE1	GLN		7		93.575	45.560	45.334	1.00	50.12		C
ATOM	3348	NE2	GLN		7		93.007	47.730	45.155	1.00	35.66		C
ATOM	3349	C	GLN		7		88.230	48.035	46.262	1.00	36.89		C
ATOM	3350	0	GLN		7		87.567	47.514	45.370	1.00	42.41		C,
ATOM	3351	N	SER	•	8		88.095	49.307	46.623	1.00	34.89		C
ATOM	3352	CA	SER		8		87.148	50.178	45.940	1.00	33.64		C
ATOM	3353	CB	SER		8		87.247	51.613	46.475	1.00	39.10		C
MOTA	3354	OG G	SER		8		86.259	51.882	47.465 44.481	1.00	33.65 36.57		Ċ
ATOM	3355 3356	C O	SER SER		8 8	•	87.564 88.751	50.141	44.180	1.00	34.54		C
MOTA	3357	И	PRO		9		86.596	50.239	43.553	1.00	45.61		C
ATOM ATOM	3357	CD	PRO		9		85.146	50.390	43.755	1.00	42.54		C
ATOM	3359	CA	PRO		9		86.946	50.207	42.128	1.00	42.76		C
ATOM	3360	CB	PRO		9		85.594	50.325	41.411	1.00	35.11		C
ATOM	3361	CG	PRO	ž	9		84.577	49.955	42.428	1.00	29.77		C
ATOM	3362	C	PRO		9	*	87.879	51.370	41.813	1.00	45.27		C '
ATOM .	3363	0	PRO		9		88.929	51.194	41.190	1.00	49.59		C
ATOM	3364		MET		10		87.486	52.561	42.254	1.00	34.14		C
ATOM	3365	CA	MET		10	4	88.292	53.749	42.041	1.00	36.35		C
ATOM	3366	CB	MET		10		87.975	54.374	40.674	1.00	51.67		C
ATOM	3367	CG	MET		10		87.958	55.908	40.628	1.00	45.29		C
ATOM	3368	SD	MET		10		86.852	56.596	39.357	1.00	41.23		C
ATOM	3369	CE	MET		10		88.067	57.323	38.239	1.00	36.20	f	C
ATOM	3370	C	MET		10		88.031	54.730	43.172	1.00	31.46		C
ATOM	3371	0	MET		10	., .	87.032	54.629	43.882	1.00	22.69		C,
ATOM	3372	N	LEU	•	11		88.962	55.661	43.344	1.00	34.82		C
ATOM	3373	CA	LEU	•	11	T	88.890	56.669	44.385	1.00	23.35		C
ATOM	3374	CB	LEU		11		89.826	56.264	45.530	1.00	20.95		C,
ATOM	3375	CG	LEU		11		89.592	54.804	45.946	1.00	18.02	ŧ	C
ATOM	3376	CD1	LEU	,	11		90.765	54.235	46.696	1.00	5.04		C
MOTA	3377	CD2	LEU	•	11		88.339	54.745	46.785	1.00	31.87		C
MOTA	3378	C	LEU		11		89.306	58.008	43.789	1.00	22.25		C
MOTA	3379	O	LEU	•	11	,	90.294	58.093	43.061	1.00	23.22		C
MOTA	3380	N	VAL	•	12		88.540	59.051	44.075	1.00	23.39	:	C
MOTA	3381	·CA	VAL		12		88.871	60.365	43.551	1.00	25.58	ı	C
MOTA	3382	CB	`VAL	•	12		87.610	61.166	43.174	1.00	37.83	ı	C
MOTA	3383	CG1	VAL	:	12		88.008	62.509	42.585	1.00	20.17	ı	C
MOTA	3384	CG2	VAL	:	12		86.771	60.387	42.173	1.00	25.83	ı	C
MOTA	3385	C	VAL	•	12		89.655	61.133	44.603	1.00	30.45		C

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ATOM	3386	0	VAL	12	89.106	61.605	45.597	1.00 47.50	·C
MOTA	3387	N	ALA	13	90.955	61.246	44.379	1.00 37.89	C
ATOM	3388	CA	ALA	13	91.820	61.943	45.307	1.00 26.16	C
MOTA	3389	CB	ALA	13	93,203	62.091	44.706	1.00 30.65	. C
ATOM	3390	C .	ALA,	13	91.241	63.309	45.615	1.00 33.79	· C
ATOM	3391	0	ALA	13	90.816	64.028	44.711	1.00 39.57	C
ATOM	3392	N	TYR	14	91,206	63.657	46.895	1.00 39.35	C
ATOM	3393	CA	TYR	14	90.711	64.959	47.306	1.00 37.04	C
ATOM	3394	CB	TYR	14	89.660	64.835	48.410	1.00 33.79	C
ATOM	3395	CG	TYR .	14	89.555	66.110	49.213	1.00 48.57	C
ATOM	3396	CD1	TYR	14	90.182	66.233	50.458	1.00 50.52	C
ATOM	3397	CE1	TYR	14	90.178	67.444	51.148	1.00 54.90	С
ATOM	3398	CD2	TYR	14	88.913	67.231	48.685	1.00 44.13	C .
ATOM.	3399	CE2	TYR	14	88.904	68.441	49.364	1.00 49.92	С
ATOM	3400	CZ	TYR	14	89.538	68.545	50.590	1.00 58.83	C
ATOM	3401	OH	TYR	14	89.536	69.761	51.240	1.00 69.05	C
ATOM	3402	C	TYR	14	91.884	65.765	47.846	1.00 39.91	C
ATOM	3403	0	TYR	14	92.626	65.283	48.703	1.00 36.85	C
ATOM	3404	N	ASP	15	92.041	66.992	47.359	1.00 34.60	С
ATOM	3405	CA	ASP	15	93.131	67.838	47.820	1.00 35.97	C
ATOM	3406	CB	ASP	15	92.958	68.141	49.307	1.00 54.21	С
ATOM	3407	CG	ASP	15	92.605	69.588	49.573	1.00 74.11	ď
ATOM	3408	OD1	ASP	15	92.300	70.322	48.604	1.00 77.84	С
ATOM	3409	OD2	ASP	15	92.634	69.985	50.758	1.00 75.11	ď
ATOM	3410	C	ASP	15	94.448	67.112	47.603	1.00 33.47	С
ATOM	3411	0	ASP	15	95.389	67.265	48.380	1.00 34.49	С
ATOM	3412	N	ASN	16	94.499	66.309	46.543	1.00 44.74	С
ATOM	3413	CA	ASN	16	95.683	65.534	46.196	1.00 48.87	C
ATOM	3414	CB	ASN	16	96.898	66.457	46.053	1.00 62.07	С
ATOM	3415	CG	ASN	16	96.840	67.292	44.793	1.00 64.94	ď
ATOM	3416	OD1	ASN	16	96.213	68.355	44.760	1.00 66.06	С
	3417	ND2	ASN	16	97.497	66.816	43.742	1.00 73.29	С
ATOM	3418	C	ASN	16	95.983	64.449	47.225	1.00 48.29	C
ATOM	3419	0	ASN	16	97.148	64.096	47.451	1.00 38.81	С
ATOM	3420	N	ALA	17	94.923	63.923	47.835	1.00 34.08	C
ATOM	3421	CA	ALA	17	95.055	62.867	48.840	1.00 29.57	C
ATOM	3422	CB	ALA	17	94.996	63.459	50.237	1.00 33.14	·C
ATOM	3423	· C	ALA	17	93.955	61.832	48.667	1.00 29.96	C
ATOM	3424	0	ALA	17	92.931	62.107	48.049	1.00 32.16	С
ATOM	3425	N	VAL	18	94.169	60.642	49.213	1.00 28.09	C
ATOM	3426	CA	VAL	18	93.188	59.568	49.111	1.00 30.54	C
ATOM	3427	CB	VAL	18	93.339	58.824	47.767	1.00 15.07	С
ATOM	3428	CG1	VAL	18	94.517	57.889	47.829	1.00 23.83	С
ATOM	3429	· CG2	VAL	18	92.086	58.054	47.448	1.00 16.29	С
ATOM	3430	C	VAL	18	93.356	58.575	50.266	1.00 33.43	С
ATOM	3431		VAL	18 .	94.314	58.660	51.029	1.00 28.92	С
ATOM	3432	N .	ASN	19	92.419	57.643	50.398	1.00 30.17	C
ATOM	3433	CA	ASN	19	92.496	56.642	51.456	1.00 28.35	С
ATOM	3434	CB	ASN	19	91.468	56.959	52.545	1.00 37.98	C
ATOM	3435	CG	ASN	19	92.105	57.540	53.794	1.00 36.06	C
ATOM	3436	OD1	ASN	19	92.991	56.923	54.385	1.00 36.77	C
ATOM	3437	ND2	ASN	19	91.659	58.732	54.205	1.00 27.02	C
ATOM	3438	C	ASN	19	92.241	55.260	50.867	1.00 28.23	C

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MOTA	3439	0 .	ASN	19	91.113	54.941	50.502	1.00	25.92	C
MOTA	3440	M	LEU	20	93.291	54.446	50.781	1.00	37.11	C
MOTA	3441	CA	LEU	20	93.192	53.097	50.204	1.00	39.33	С
ATOM	3442	CB	LEU	20	94.382	52.830	49.284	1.00	52.73	С
MOTA	3443	CG	LEU	20 ;	94,409	53.492	47.913	1.00	59.34	Ĉ
ATOM	3444	CD1	LEU ·	20	95.375	54.657	47.953	1.00	54.35	. С
MOTA	3445	CD2	LEU	20	94.826	52.478	46.855	1.00	58.17	С
MOTA	3446	C	LEU	20	93.122	51.946	51.202	1.00	24.88	С
ATOM	3447	0	LEU	20	94.141	51.349	51.532	1.00	27.29	C
MOTA	3448	N	SER	21	91.926	51.619	51.670	1.00	24.25	С
ATOM	3449	CA	SER	21	91.795	50.515	52.601	1.00	32.93	C
MOTA	3450	CB	SER	21.	90.474	50.603	53.357	1.00	22.84	С
MOTA	3451	OG	SER	21	90.626	50.123	54.682	1.00	42.82	C
MOTA	3452	C	SER	21	91.834	49.250	51.760	1.00	36.87	C
ATOM	3453	0	SER	21	91.633	49.308	50.551	1.00	50.83	С
ATOM	3454	N	CYS	22	92.098	48.109	52.384	1.00	41.84	С
ATOM	3455	CA	CYS	22	92.142	46.858	51.636	1.00	34.97	С
ATOM	3456	С	CYS	22	91.519	45.728	52.420	1.00	29.54	C
ATOM	3457	0	CYS	22	92.086	45.250	53.400	1.00	31.51	С
ATOM	3458	CB	CYS	22	93.578	46.504	51.294	1.00	44.42	C
ATOM	3459	SG	CYS	22	94.382	47.674	50.162	1.00	54.15	С
ATOM	3460	N	LYS	23	90.339	45.312	51.983	1.00	9.94	С
ATOM	3461	CA	LYS	23	89.630	44.234	52.639	1.00	27.48	С
ATOM	3462	CB	LYS	23	88.196	44.149	52.099	1.00	45.60	С
ATOM	3463	CG	LYS	23	87.083	44.123	53.160	1.00	46.91	C
ATOM	3464	CD -	LYS	23	85.742	44.572	52.558	1.00	49.03	C
ATOM	3465	CE	LYS	23	84.537	43.911	53.219	1.00	44.60	С
ATOM	3466	NZ	LYS	23	83.321	43.966	52.347	1.00	31.56	C
ATOM	3467	C	LYS	23 .	90.373	42.933	52.354	1.00	28.04	C
ATOM	3468	0	LYS	23	90.727	42.651	51.209	1.00	27.74	C
ATOM	3469	N	TYR	24	90.616	42.154	53.404	1.00	48.19	C
MOTA	3470	CA.	TYR	24	91.305	40.869	53.279	1.00	51.31	C
ATOM	3471	CB	TYR	24	92.585	40.864	54.121	1.00	33.41	C
ATOM	3472	CG	TYR	24	93.582	41.914	53.708	1.00	28.69	C
ATOM	3473	CD1	TYR	24	94.190	41.867	52.454	1.00	41.70	C
ATOM	3474	CE1	TYR	24	95.089	42.846	52.049	1.00	20.51	C
ATOM	3475	CD2	TYR	24	93.901	42.971	54.554	1.00	29.67	C
ATOM	3476	CE2	TYR	24	94.803	43.960	54.159	1.00	21.03	С
ATOM	3477	CZ	TYR	24	95.389	43.889	52.905	1.00	18.10	С
ATOM	3478	OH	TYR	24	96.263	44.862	52.495	1.00	37.76	С
ATOM	3479	C	TYR	24	90.403	39.736	53.749	1.00	47.73	C
ATOM	3480	0	TYR	24	89.264	39.957	54.151	1.00	49.24	C
ATOM	3481	N	SER	25	90.920	38.518	53.690	1.00	57.38	C
ATOM	3482	CA	SER	25	90.175	37.353	54.146	1.00	60.28	C
ATOM	3483	CB	SER	25	89.888	36.407	52.975	1.00	59.25	C
ATOM	3484	OG	SER	25 .	91.068	36.142	52.238	1.00	69.79	C
ATOM	3485	C	SER	25	91.076	36.668	55.164	1.00	54.52	С
ATOM	3486	0	SER	25	91.290	35.455	55.108	1.00	60.55	С
ATOM	3487	N	TYR	26	91.606	37.458	56.096		43.18	C
ATOM	3488	CA	TYR	26	92.516	36.933	57.101	1.00	31.88	C
ATOM	3489	CB	TYR	26	93.949	36.995	56.566	v	26.62	С
ATOM	3490	CG	TYR	26	94.845	35.878	57.060		37.63	С
ATOM	3491	CD1	TYR	26	95.606	36.026	58.220		43.69	C
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ATOM	3492	CE1	TYR	26	96.443	35.003	58.673	1.00 50.	14 C
MOTA	3493	CD2	TYR	26	94.941	34.677	56.363	1.00 43.	*
MOTA	3494	CE2	TYR	26	95.776	33.646	56.809	1.00 62.	28 C
MOTA	3495	CZ	TYR	26	96.524	33.816	57.964	1.00 56.	86 C
ATOM	3496	OH	TYR	26	97.352	32.801	58.404	1.00 54.	48 C
MOTA	3497	C	TYR	26	92.455	37.637	58.451	1.00 30.	34 C
ATOM	3498	0	TYR	26	92.275	38.851	58.518	1.00 12.	16 C
ATOM	3499	N	ASN	27	92.626	36.832	59.504	1.00 35.	16 C
MOTA	3500	CA	ASN	27	92.639	37.230	60.920	1.00 43.	53 C
MOTA	3501	CB	ASN	27	94.092	37.461	61.380	1.00 44.	74 C
ATOM	3502	CG	ASN	27	94.595	38.869	61.095	1.00 54.	71 C
ATOM	3503	OD1	ASN	27	93.890	39.691	60.503	1.00 49.	86 C
ATOM	3504	ND2	ASN	27	95.833	39.153	61.521	1.00 38.	35 C
ATOM	3505	C	ASN	27	91.760	38.379	61.413	1.00 52.	07 C
ATOM	3506	0	ASN	27	91.255	39.159	60.582	1.00 64.	58 C
ATOM	3507	\mathbf{T} O	ASN	27	91.583	38.478	62.651	1.00 38.	64 C
MOTA	3508	CB	SER	30	98.029	39.101	66.273	1.00 38.	67 C
ATOM	3509	OG	SER	30	99.164	39.940	66.371	1.00 28.	74 C
ATOM	3510	C	SER	30	99.198	37.741	64.527	1.00 48.	62 C
MOTA	3511	0	SER	30	99.534	36.748	65.163	1.00 42.	19 C
MOTA	3512	N	SER	30	96.758	37.537	64.847	1.00 40.	61 C
ATOM	3513	CA	SER	30	97.910	38.480	64.881	1.00 46.	89 C
ATOM	3514	N	ARG	31	, 99.906	38.226	63.505	1.00 52.	76 · C
ATOM	3515	CA	ARG	31	101.156	37.606	63.056	1.00 48.	62 · C
ATOM	3516	CB	ARG	31	100.864	36.509	62.014	1.00 48.	21 C
ATOM	3517	CG	ARG	31	99.390	36.316	61.654	1.00 45.	
MOTA	3518	CD	ARG	31	99.123	34.913	61.098	1.00 45.	
ATOM	3519	NE	ARG	31	98.202	34.159	61.946	1.00 56.	
ATOM	3520	CZ	ARG	31	97.819	32.904	61.723	1.00 60.	·
MOTA	3521	NH1	ARG	31	98.273	32.238	60.666	1.00 53.	•
ATOM	3522	NH2	ARG	31	96.980	32.312	62.565	1.00 65.	
MOTA	3523	C	ARG	31	102.140	38.620	62.457	1.00 42.	
MOTA	3524	0	ARG	31	102.024	39.821	62.696	1.00 37.	
MOTA	3525	N	GLU	32	103.109	38.119	61.688,		
MOTA	3526	CA	GLU	32	104.114	38.959		1.00 28.	
ATOM	3527	CB	GLU	32	105.510	38.366	61.211	1.00 35.	
ATOM	3528	CG	GLU	32	106.639	39.289	60.762	1.00 44.	
ATOM	3529	CD	GLU	32	107.993	38.584	60.704	1.00 47.	
ATOM	3530	OE1	GLU	32	108.183	37.588	61.436	1.00 50.	
ATOM	3531	OE2	GLU	32	108.870	39.024	59.931	1.00 43.	
ATOM	3532	C	GLU	32	103.777	39.047	59.550	1.00 32.	
ATOM	3533	0	GLU	32	103.876	38.061	58.815	1.00 19.	
ATOM	3534	N	PHE	33	103.394	40.244	59.122	1.00 41.4	
ATOM	3535	CA	PHE	33	102.989	40.488	57.747	1.00 35.0	
ATOM	3536	CB	PHE	33	101.494	40.691	57.715	1.00 26.	
ATOM	3537	CG	PHE	33	101.065	41.944	58.408	1.00 24.	
ATOM	3538	CD1	PHE	33	101.369	43.192	57.861	1.00 23.4	
ATOM	3539	CD2	PHE	33	100.374	41.889	59.611	1.00 15:0	
ATOM	3540	CE1	PHE	33 .	100.989	44.367	58.496	1.00 28.0	
ATOM	3541	CE2	PHE	33	99.984	43.063	60.260	1.00 24.	
ATOM	3542	CZ	PHE	33	100.292	44.304	59.703	1.00 31.3	
ATOM	3543	C	PHE	33	103.640	41.716	57.121	1.00 34.	
MOTA	3544	0	PHE	33	104,134	42.613	57.813	1.00 21.	74 C

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ATOM	3545	N	ARG	34	103.564	41.771	55.797	1.00 28.28	C
ATOM	3546	CA	ARG	34	104.145	42.864	55.045	1.00 21.13	C
MOTA	3547	CB	ARG	34	105.469	42.413	54.437	1.00 12.61	ď
MOTA	3548	CG	ARG	34	106.189	43.483	53.643	1.00 19.39	C
ATOM	3549	CD	ARG	34	106.709	42.916	52.339	1.00 18.93	C,
ATOM	3550	NE	ARG	34	108.026	43.440	51.995	1.00 36.83	C
ATOM	3551	CZ	ARG	34	108.251	44.344	51.045	1.00 40.83	C
ATOM	3552	NH1	ARG	34	107.239	44.825	50.340	1.00 45.97	C
ATOM	3553	NH2	ARG	34	109.490	44.752	50.785	1.00 38.52	C
ATOM	3554	С	ARG	34	103.202	43.309	53.940	1.00 32.95	C
ATOM	3555	0	ARG	34	103.239	42.779	52.831	1.00 41.93	C.
ATOM	3556	N	ALA	35	102.362	44.294	54.239	1.00 34.63	C
ATOM	3557	CA	ALA	35	101.416	44.798	53.251	1.00 26.09	C
ATOM	3558	CB	ALA	35	100.381	45.657	53.921	1.00 26.37	C
ATOM	3559	C	ALA	35	102.134	45.599	52.173	1.00 28.19	C
MOTA	3560	0	ALA	35	103.201	46.163	52.414	1.00 19.20	C
MOTA	3561	N	SER	36	101.545	45.641	50.980	1.00 36.87	C
MOTA	3562	CA	SER	36	102.136	46.374	49.863	1.00 39.36	C
MOTA	3563	CB	SER	36	103.172	45.488	49.160	1.00 51.82	C
ATOM	3564	OG	SER	36	103.705	44.516	50.050	1.00 62.97	C
MOTA	3565	C	SER	36	101.099	46.886	48.847	1.00 32.13	C
MOTA	3566	0	SER	36	100.092	46.238	48.575	1.00 28.44	C
MOTA	3567	N	LEU	37	101.364	48.069	48.304	1.00 34.51	C
MOTA	3568	CA	LEU	37	100.496	48.705	47.320	1.00 31.61	C
ATOM	3569	CB	LEU	37	99.897	49.987	47.895	1.00 36.64	C
MOTA	3570	CĠ	LEU	37	98.943	50.801	47.023	1.00 21.97	C
MOTA	3571	CD1	LEU	37	97.533	50.720	47.578	1.00 21.64	C
MOTA	3572	CD2	LEU	37	99.412	52.231	46.991	1.00 26.43	C
MOTA	3573	C	LEU	37	101.393	49.042	46.148	1.00 28.60	C
MOTA	3574	0	LEU	37	102.341	49.811	46.295	1.00 35.19	C
MOTA	3575 🗓	\mathbf{N}	HIS	38	101.112	48.454	44.993	1.00 22.34	C
ATOM	3576	CA	HIS	38	101.935	48.694	43.816	1.00 21.00	C
MOTA	3577	CB	HIS	38	102.418	47.370	43.232	1.00 29.80	C
MOTA	3578	CG	HIS	38	103.038	46.464	44.248	1.00 41.65	C
MOTA	3579	CD2	HIS	38	104.324	46.102	44.458	1.00 36.66	· C
MOTA	3580	ND1	HIS	38	102.296	45.819	45.218	1.00 51.35	C
ATOM	3581	CEl	HIS	38	103.102	45.102	45.978	1.00 45.79	C
MOTA	3582	NE2	HIS	38	104.337	45.256	45.539	1.00 50.11	C
MOTA	3583	C -	HIS	38	101.138	49.458	42.794	1.00 20.21	, C
ATOM	3584	0	HIS	38	99.935	49.263	42.679	1.00 24.62	C
ATOM	3585	N	LYS	39	101.807	50.334	42.055	1.00 17.62	ď
ATOM	3586	CA	LYS	39	101.135	51.154	41.065	1.00 28.42	C
ATOM	3587	CB	LYS	39	101.458	52.627	41.334	1.00 33.83	C
MOTA	3588	CG .	LYS	39	100.938	53.579	40.281	1.00 47.76	C
MOTA	3589,	CD	LYS	39	102.046	54.496	39.767	1.00 56.33	C
ATOM	3590	CE	LYS	39	101.922	54.727	38.264	1.00 52.05	C
MOTA	3591	NZ	LYS	39	101.573	56.133	37.920	1.00 39.26	C
MOTA	3592	C	LYS	39	101.527	50.784	39.644	1.00 37.38	C
MOTA	3593	0	LYS	39	102.715	50.697	39.323	1.00 38.26	C
MOTA	3594	N	GLY	40	100.528	50.559	38.793	1.00 33.72	C
MOTA	3595	CA	GLY	40	100.819	50.230	37.412	1.00 30.90	C
MOTA	3596	C	GLY	40	100.183	48.957	36.913	1.00 33.65	C
MOTA	3597	0	GLY	40	100.025	47.997	37.665	1.00 26.93	C

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	ATOM	3598	Й	LEU	41	99.819	48.962	35.634	1.00 48.13	· C
	ATOM	3599	CA	LEU	41	99.196	47.809	34.988	1.00 43.35	C
	ATOM	3600	CB	LEU	41	98.598	48.211	33.633	1.00 41.37	C
	ATOM	3601	CG ·	LEU	41	97.256	47.613	33.178	1.00 50.66	C
	ATOM	3602	CD1	LEU	41	96.622	46.783	34.283	1.00 41.32	Ċ
	ATOM	3603	CD2	LEU	41	96.324	48.742	32.756	1.00 36.16	C
	ATOM	3604	С	LEU	41	100.270	46.758	34.791	1.00 44.95	C
	ATOM	3605	0	LEU	41	99.976	45.585	34.577	1.00 48.29	C
	ATOM	3606	N	ASP	42	101.522	47.197	34.841	1.00 51.52	C
	ATOM	3607	CA	ASP	42	102.648	46.285	34.713	1.00 53.82	C
	ATOM	3608	CB	ASP	42	103.666	46.804	33.690	1.00 44.60	С
	ATOM	3609	CG	ASP	42	104.352	48.090	34.125	1.00 49.55	C.
	ATOM	3610		ASP	42	103.874	48.765	35.063	1.00 40.26	С
	ATOM	3611	OD2	ASP	42	105.385	48.427	33.510	1.00 48.33	С
	ATOM	3612	C	ASP	42	103.249	46.241	36.106	1.00 57.65	С
	ATOM	3613	0	ASP	42	104.394	45.836	36.298	1.00 57.61	C
	ATOM	3614	N ·	SER	43	102.433	46.679	37.065	1.00 57.54	C
	ATOM	3615	CA	SER	43	102.767	46.741	38.486	1.00 56.75	C
	ATOM	3616	CB	SER	43	102.299	45.467	39.177	1.00 40.78	C
	ATOM	3617	OG	SER	43	100.896	45.502	39.359	1.00 32.86	C
	ATOM	3618	C	SER	43	104.234	46.995	38.803	1.00 59.27	С
	ATOM	3619	0	SER	43	104.795	46.413	39.732	1.00 57.66	С
	ATOM	3620	N	ALA	44	104.847	47.884	38.033	1.00 54.64	С
	ATOM	3621	CA	ALA	44	106.244		38.224	1.00 41.67	С
	ATOM	3622	CB	ALA	44	106.654	49.295	37.239	1.00 41.38	C
	ATOM	3623	C	ALA	44	106.514	48.679	39.646	1.00 42.01	C
	ATOM	3624	0	ALA	44	107.073	47.935	40.449	1.00 48.39	С
**	ATOM	3625	N	VAL	45	106.083	49.904	39.943	1.00 40.52	C
	ATOM	3626	CA	VAL	45	106.290	50.563	41.239	1.00 34.97	C
	ATOM	3627	CB	VAL	45	106.036	52.073	41.094	1.00 27.80	С
:	ATOM	3628	CG1	VAL	45	106.126	52.753	42.441	1.00 32.20	C
	ATOM	3629	CG2	VAL	45	107.036	52.674	40.126	1.00 35.71	С
	ATOM	3630	C	VAL	45	105.526	50.100	42.489	1.00 35.47	C
	ATOM	3631	0	VAL	45	104.307	49.956	42.462	1.00 45.80	ď
ı	ATOM	3632	N	GLU	46	106.259	49.893	43.585	1.00 39.87	ď
	MOTA	3633	CA	GLU	46	105.666	49.503	44.868	1.00 41.71	C
	ATOM	3634	CB.	GLU	46	106.546	48.488	45.615	1.00 50.85	C
	ATOM	3635	CG	GLU	46	106.163	48.251	47.094	1.00 34.64	C
	ATOM	3636	CD	GLU	46	106.638	46.895	47.637	1.00 57.55	C
	ATOM	3637	OE1		46	107.869	46.712	47.809	1.00 47.66	C
	ATOM	3638	OE2	GLU	46	105.783	46.014	47.893	1.00 29.27	C
	ATOM	3639	C	GLU	46	105.575	50.791	45.680	1.00 37.48	С
	ATOM	3640	0	GLU	46	106.530	51.189	46.338	1.00 43.67	С
	ATOM	3641	· N	VAL	47	104.418	51.433	45.614	1.00 25.13	C
	ATOM	3642	CA	VAL	47	104.173	52.692	46.297	1.00 15.83	C
	ATOM	3643	CB	VAL	47	102.736	53.146	46.037	1.00 19.37	C
	ATOM	3644	CG1	VAL	47	102.428	54.405	46.826	1.00 28.90	,C
	MOTA	3645	CG2	VAL	47	102.543	53.374	44.547	1.00 26.86	C
	ATOM	3646	C	VAL	47	104.437	52.717	47.800	1.00 29.17	C
	ATOM	3647	0	VAL	47	105.070	53.641	48.310	1.00 31.30	С
	ATOM	3648	N	CYS	48	103.952	51.709	48.512	1.00 40.43	C
	ATOM	3649	CA	CYS	48	104.142	51.665	49.955	1.00 37.33	C
	ATOM	3650	C	CYS	48	104.145	50.246	50.495	1.00 27.79	C
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ATOM	. 3651	0	CYS	48		103.618	49.331	49.864	1.00	20.24	C
ATOM	3652	CB	CYS	48		103.035	52.459	50.644	1.00	57.93	C
ATOM	3653	SG	CYS	48		103.314	52.822	52.407	1.00	69.94	С
MOTA	3654	\mathbf{N}	VAL	49	· ·	104.747	50.070	51.664	1.00	18.58	. C
ATOM	3655	CA	VAL	49		104.802	48.764	52.290	1.00	20.44	С
ATOM	3656	СВ	VAL	49		106.139	48.030	51.966	1.00	27.56	C
MOTA	3657	CG1	VAL	49		107.042	48.931	51.131	1.00	18.34	C
ATOM	3658	CG2	VAL	49		106.851	47.592	53.249	1.00	17.63	C
ATOM	3659	C	VAL	49		104.654	48.926	53.794	1.00	33.14	C
ATOM	3660	0	VAL	49		105.537	49.471	54.455	1.00	29.92	C
ATOM	3661	N	VAL	50		103.523	48.467	54.324	1.00	41.12	С
ATOM	3662	CA	VAL	50		103.255	48.539	55.759	1.00	44.37	С
MOTA	3663	CB	VAL	50		101.796	48.932	56.031	1.00	48.04	C
ATOM	3664	CG1	VAL	50		101.486	48.786	57.511	1.00	45.70	С
ATOM	3665	CG2	VAL	50		101.562	50.367	55.576	1.00	35.76	C
ATOM	3666	C	VAL	50		103.553	47.176	56.385	1.00	38.20	C
ATOM	3667	0	VAL	50		102.899	46.176	56.085	1.00	36.51	C
MOTA	3668	N	TYR	51		104.543	47.146	57.264	1.00	25.60	C
ATOM	3669	CA	TYR	51		104.957	45.898	57.879	1.00	34.11	C
ATOM	3670	CB	TYR	51		106.479	45.779	57.799	1.00	34.41	C
ATOM	3671	CG	TYR	51		107.060	44.744	58.724	1.00	31.19	C
ATOM	3672	CDI	TYR	51		107.617	45.109	59.944	1.00	38.77	C
MOTA	3673	CE1	TYR	51		108.122	44.153	60.822	1.00	44.07	, C
MOTA	3674	CD2	TYR	51		107.025	43.396	58.395	1.00	33.29	C
ATOM	3675	CE2	TYR	51		107.525	42.432	59.265	1.00	41.62	C
ATOM	3676	CZ	TYR	51	2 4	108.068	42.818	60.477	1.00	39.08	C
ATOM	3677	OH	TYR	51	4	108.511	41.867	61.364	1.00	47.15	C
ATOM	3678	C	TYR	51		104.507	45.729	59.315	1.00	33.68	C
ATOM	3679	0	TYR	51		104.696	46.613	60.145	1.00	23.59	C
ATOM	3680	И	GLY	52		103.927	44.571	59.603	1.00	29.01	C
ATOM	3681	CA	GLY	52		103.459	44.300	60.947	1.00	30.05	C
MOTA	3682	C	GLY	. 52	1	104.067	43.041	61.527	1.00	39.73	C
MOTA	3683	0	GLY	52		104.393	42.096	60.806	1.00	40.35	C
ATOM	3684	N	ASN	53		104.224	43.032	62.843	1.00	46.66	C ·
ATOM	3685	CA	ASN	53		104.798	41.888	63.537	1.00	57.56	C
ATOM	3686	CB	ASN	53	•	106.308	42.073	63.721	1.00	32.73	C
ATOM	3687	CG	ASN	53	,	106.971	40.851	64.322	1.00	30.74	C
MOTA	3688	OD1	ASN	53		106.474	39.728	64.185	1.00	25.99	. C
ATOM	3689	ND2	ASN	53		108.099	41.059	64.995	1.00	35.70	C
MOTA	3690	C	ASN	53		104.141	41.729	64.897	1.00	63.15	C
MOTA	3691	Ο,	ASN	53		104.709	42.114	65.918	1.00	67.81	C
MOTA	3692	N	TYR	54		102.941	41.159	64.906	1.00	66.70	С
MOTA	3693	CA	TYR	54		102.213	40.953	66.149	1.00	70.87	C _
MOTA	3694	CB	TYR	54		103.004	40.008	67.072	1.00	60.20	C
ATOM	3695	CG	TYR	54		103.185	38.604	66.521	1.00	54.18	C
MOTA	3696	CD1	TYR	54		104.380	38.215	65.923	1.00	49.72	C
ATOM	3697	CE1	TYR	54		104.538	36.931	65.393	1.00	51.50	С
MOTA	3698	CD2	TYR	54		102.149	37.672	66.579	1.00	63.25	C
ATOM	3699	CE2	TYR	54		102.297	36.386	66.052	.1.00	53.22	С
ATOM	3700	CZ	TYR	54		103.489	36.025	65.461	1.00	51.26	C
ATOM	3701	OH	TYR	54		103.625	34.761	64.931	1.00	41.36	С
MOTA	3702	C	TYR	54		102.018	42.313	66.811		75.80	C
MOTA	3703	0	TYR	54		101.118	43.072	66.443	1.00	70.77	С

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ATOM	3704	N	SER	55	102.870	42.617	67.784	1.00 83.17	: C
ATOM	3705	CA	SER	55	102.805	43.892	68.483	1.00 89.21	C
ATOM	3706	CB	SER	55	103.373	43.750	69.896	1.00 89.77	· C
ATOM	3707	OG	SER	55	102.332	43.662	70.853	1.00 90.69	C
ATOM	3708	C .	SER	55 [°]	103.617	44.916	67.695	1.00 90.09	C
ATOM	3709	0	SER	55	103.181	45.378	66.639	1.00 92.24	, C
ATOM	3710	N	GLN	56	104.796	45.251	68.218	1.00 90.35	С
ATOM	3711	CA	GLN	56	105.715	46.207	67.600	1.00 93.42	C
ATOM	3712	CB	GLN	56	106.882	45.448	66.957	1.00 91.24	C
ATOM	3713	CG	GLN	56	107.492	44.372	67.861	1.00 94.20	С
ATOM	3714	CD	GLN	56	108.069	43.192	67.088	1.00 99.99	С
ATOM	3715	OE1	GLN	56	108.128	42.066	67.595	1.00 87.06	G,
ATOM	3716	NE2	GLN	56	108.500	43.446	65.854	1.00 99.99	. C
ATOM	3717	C	GLN	56	105.040	47.121	66.572	1.00 96.11	C
ATOM	3718	0	GLN	56	104.866	46.744	65.413	1.00 99.98	С
ATOM	3719	N	GLN	57	104.670	48.323	67.013	1.00 90.45	С
ATOM	3720	CA	GLN	57	103.995	49.318	66.177	1.00 83.45	С
ATOM	3721	CB	GLN	. 57	104.417	50.732	66.589	1.00 85.60	С
ATOM	3722	CG	GLN	57	104.367	50.991	68.084	1.00 89.34	С
ATOM	3723	CD	GLN	57	105.744	50.966	68.718	1.00 87.16	C
ATOM	3724	OE1	GLN	57	106.497	51.937	68.635	1.00 76.99	С
ATOM	3725	NE2	GLN	5 <i>7</i> -	106.080	49.849	69.355	1.00 90.12	C
ATOM	3726	C	GLN	5 <i>7</i>	104.185	49.175	64.669	1.00 80.35	C
ATOM	3727	0	GLN	57 ·	105.278	48.877	64.182	1.00 77.96	C
ATOM	3728	N	LEU	58	103.095	49.401	63.943	1.00 76.47	C
ATOM	3729	CA	LEU	58	103.077	49.331	62.487	1.00 61.35	C
ATOM	3730	CB	LEU	58	101.723	49.838	61.972	1.00 52.59	C
ATOM	3731	CG	LEU	58	100.956	49.130	60.845	1.00 50.02	C
ATOM	3732	CD1	LEU	58	100.916	47.634	61.070	1.00 55.58	C
ATOM	3733	CD2	LEU	58	99.535	49.671	60.794	1.00 39.64	C
ATOM	3734	C	LEU	58	104.209	50.181	61.906	1.00 54.39	C .
ATOM	3735	0	LEU	58	104.387	51.345	62.284	1.00 51.09	C
ATOM	3736	N .	GLN	59	104.976	49.589	60.997	1.00 51.81	C
ATOM	3737	CA	GLN	5 <i>9</i>	106.080	50.290	60.346	1.00 46.97	C
ATOM	3738	CB	GLN	5 <i>9</i>	107.394	49.516	60.524	1.00 35.66	C
ATOM	3739	CG	GLN	59 ·	108.469	50.260	61.308	1.00 32.42	C
ATOM	3740	CD	GLN ·	59	109.327	49.340	62.171	1.00 53.43	C
ATOM	3741	OE1	GLN	5 <i>9</i>	110.198	49.799	62.912	1.00 50.95	C
ATOM -	3742	NE2		5 <i>9</i>	109.082	48.037	62.079	1.00 46.72	· C
ATOM	3743	C	GLN	5 <i>9</i>	105.748	50.417	58.859	1.00 43.43	C
ATOM	3744	0	GLN	59 ·	105.697	49.422	58.138	1.00 42.60	C
ATOM	3745	N	VAL	60	105.505	51.645	58.412	1.00 40.75	C
	3745	CA	VAL	60	105.172	51.907	57.018	1.00 39.80	C
ATOM ATOM		CB	VAL	60	103.828	52.659	56.896	1.00 26.19	C
	3747		VAL	60	103.878	53.955	57.678	1.00 21.41	C
ATOM	3748	CG1			103.578	52.946	55.448	1.00 27.26	C
ATOM	3749 3750	CG2	VAL .	60 60	105.526	52.745	56.371	1.00 27.20	C
ATOM	3750 3751	C	VAL VAL	60	106.267	53.727	56.950	1.00 41.05	C
ATOM	3751 3752	N	TYR	60 61	106.733	52.349		1.00 31.58	C
ATOM	3752 3753		TYR	61	100.032	53.086	54.477	1.00 37.83	C
ATOM ATOM	3753 3754	CA CB	TYR	61	107.731	52.575	54.861	1.00 23.83	C
	3755	CG	TYR	61	109.116	51.237	54.274	1.00 12.00	C
ATOM			TYR	61	109.496	50.053	54.953	1.00 18.31	G.
ATOM	3756	CD1	TTL	ŮТ.	107.210	20.022	J J. J. J	T.00 ZZ.ZJ	

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	ATOM	3757	CE1	TYR	61	109.599	48.819	54.439	1.00	33.05	, , C
	ATOM	3758	CD2	TYR	61	110.173	51.150	53.057	1.00	38.49	. C
	ATOM	3759	CE2	TYR	61	110.562	49.918	52.533	1.00	23.48	Ĉ
	MOTA	3760	CZ	TYR	61	110.269	48.758	53.231	1.00	29.34	C
	ATOM	3761	OH	TYR	61	110.627	47.535	52.714	1.00	30.14	C
	MOTA	3762	C	TYR	61	107.540	52.981	52.986	1.00	35.71	С
	ATOM	3763.	٠0	TYR	61	106.694	52.214	52.513	1.00	35.76	C
	ATOM	3764	N	SER	62	108.322	53.775	52.258	1.00	39.08	C
~	ATOM	3765	CA	SER	62	108.268	53.813	50.805	1.00	39.42	C
	MOTA	3766	CB	SER	62	107.247	54.857	50.345	1.00	32.31	С
	ATOM	3767	OG	SER	62	107.120	54.853	48.932	1.00	23.48	С
	ATOM	3768	C	SER	62	109.643	54.137	50.220	1.00	45.43	С
	MOTA	3769	0	SER	62	110.287	55.116	50.601	1.00	42.20	C
	ATOM	3770	N	LYS	63	110.094	53.302	49.294	1.00	50.45	C
	ATOM	3771	CA	LYS	63	111.388	53.499	48.655	1.00	44.30	C
	ATOM	3772	CB	LYS	63	112.040	52.136	48.373	1.00	41.16	C
	ATOM	3773	CG -	LYS	63	113.045	51.676	49.431	1.00	41.13	C
		3774	CD	LYS	63	112.720	50.288	49.969	1.00	36.52	С
	ATOM	3775	CE	LYS	63	113.769	49.809	50.972	1.00	27.51	C
	ATOM	3776	NZ	LYS	63	114.917	49.099	50.322	1.00	14.01	C
	MOTA	3777	С	LYS	63	111.173	54.243	47.343	1.00	40.39	С
	ATOM	3778	0	LYS	63	112.079	54.322	46.515	1.00	43.49	С
	ATOM	3779	N	THR	64	109.977	54.802	47.166	1.00	38.77	C
	ATOM	3780	CA	THR	64	109.635	55.496	45.926	1.00	33.97	C
	ATOM	3781	CB	THR	64	108.407	54.837	45.264	1.00	45.65	С
	ATOM	3782	OG1	THR	64	107.445	54.502	46.272	1.00	61.07	C
	ATOM	3783	CG2	THR	64	108.811	53.576	44.520	1.00	45.91	C
	ATOM	3784	C	THR	64	109.360	56.988	46.033	1.00	33.47	С
	ATOM	3785	0	THR	64	109.122	57.651	45.023	1.00	25.44	C
•	ATOM	3786	Ν.	GLY	65	109.375	57.525	47.244	1.00	35.21	С
	ATOM	3787	CA	GLY	65	109.119	58.946	47.383	1.00	35.72	С
	ATOM	3788	С	GLY	65	107.644	59.286	47.468	1.00	35.69	C
	ATOM	3789	0	GLY	65	107.198	60.317	46.970	1.00	41.32	C
	ATOM	3790	N	PHE	66	106.881	58.405	48.100	1.00	31.14	C
	ATOM	3791	CA	PHE	66	105.454	58.616	48.280	1.00	22.44	C
	ATOM	3792	CB	PHE	66	104.680	57.350	47.914	1.00	15.68	. ·
	ATOM	3793	CG	PHE	66	104.307	57.256	46.463	1.00	27.36	C
:	ATOM	3794	CD1	PHE	66	105.243	56.859	45.514	1.00	38.42	C
	ATOM	3795	CD2	PHE	66	103.009	57.536	46.042	1.00	42.24	C
,	ATOM	3796	CE1	PHE	66	104.889	56.738	44.159	1.00	42.03	C
	ATOM	3797	CE2	PHE	66	102.648	57.419	44.694	1.00	38.62	С
	ATOM	3798	CZ	PHE	66	103.590	57.018	43.750	1.00	28.00	C
,	ATOM	3799	C ,	PHE	66	105.238	58.921	49.758	1.00	29.60	C
	ATOM	3800	0	PHE	66	105.701	58.176	50.622	1.00	28.41	C
	ATOM	3801	N	ASN	67	104.569	60.028	50.053	1,00	29.26	C
7	ATOM	3802	CA	ASN	67	104.289	60.375	51.436	1.00	28.71	С
*	ATOM	3803	CB	ASN	67	103.776	61.814	51.516	1.00	44.50	C
	MOTA	3804	CG	ASN	67	103.832	62.385	52.923	1.00	56.37	C
	MOTA	3805	OD1	ASN	67	103.890	63.603	53.110	1.00	55.38	C
	ATOM	3806	ND2	ASN	67	103.816	61.507	53.922	1.00	49.90	C
	ATOM	3807	C	ASN	67	103.208	59.390	51.891	1.00	30.16	C
79	ATOM	3808	0	ASN	67	102.018	59.698	51.893	1.00	22.60	С
	ATOM	3809	\mathbf{N}	CYS	68	103.627	58.190	52.276	1.00	45.93	C
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ATOM	3810	CA	CYS	68	102.678	57.165	52.691	1.00 37.84	C
MOTA	3811	C	CYS	68	102.480	56.998	54.198	1.00 40.89	G.
ATOM	3812	0	CYS	68	103.414	57.122	54.986	1.00 26.35	· C .
MOTA	3813	CB	CYS	68	103.087	55.824	52.089	1.00 23.40	C
MOTA	3814	SG	CYS	68	102.108	54.426	52.713	1.00 53.33	С
ATOM	3815	N	ASP	69	101.243	56.700	54.579	1.00 44.34	C
MOTA	3816	CA	ASP	69	100.880	56.482	55.974	1.00 40.80	С
ATOM	3817	CB	ASP	69	100.101	57.683	56.515	1.00 56.37	С
MOTA	3818	CG	ASP	69	100.821	59.001	56.287	1.00 59.33	C
ATOM	3819	OD1	ASP	69	100.303	59.840	55.520	1.00 66.37	C
ATOM	3820	OD2	ASP	69	101.902	59.200	56.877	1.00 68.80	C
ATOM	3821	C	ASP	69	100.001	55.240	56.013	1.00 32.24	C
ATOM	3822	0	ASP	69	99.172	55.051	55.128	1.00 33.63	C
ATOM	3823	N	GLY	70	100.175	54.395	57.026	1.00 34.87	С
MOTA	3824	CA	\mathtt{GLY}	70	99.369	53.184	57.107	1.00 28.23	C
MOTA	3825	C	GLY	70	98.691	52.933	58.444	1.00 28.75	С
MOTA	3826	0	GLY	70	99.260	53.198	59.501	1.00 34.76	C
MOTA	3827	N	LYS	71	97.468	52.416	58.394	1.00 40.41	C
ATOM	3828	CA	LYS	71	96.697	52.123	59.599	1.00 49.78	C
MOTA	3829	CB	LYS.	71	95.522	53.095	59.714	1.00 57.09	C
MOTA	3830	CG	LYS	71	95.747	54.285	60.629	1.00 56.31	С
MOTA	3831	CD	LYS	71	94.477	55.139	60.720	1.00 55.32	С
MOTA	3832	CE	LYS	71	94.459	56.004	61.984	1.00 59.27	C
MOTA	3833	NZ	LYS	71	93.094	56.536	62.310	1.00 33.49	C
MOTA	3834	С	LYS	71	96.160	50.690	59.553	1.00 51.01	С
MOTA	3835	0	LYS	71	95.553	50.274	58.568	1.00 42.24	С
MOTA	3836	N	LEU	72	96.373	49.940	60.628	1.00 51.79	C
MOTA	3837	CA	LEU	72	95.907	48.564	60.684	1.00 61.74	C
MOTA	3838	CB	LEU	72	96.773	47.760	61.650	1.00 62.34	С
ATOM	3839	CG	LEU	72	97.284	46.425	61.103	1.00 66.36	C
MOTA	3840	CD1	LEU	72	98.165	45.754	62.147	1.00 68.74	С
MOTA	3841	CD2	LEU	72	96.107	45.527	60.736	1.00 53.65	C
ATOM	3842	C'	LEU	72	94.436	48.447	61.090	1.00 73.73	С
ATOM	3843	0	LEU	72	93.860	49.374	61.663	1.00 88.59	C
MOTA	3844	N	GLY	73	93.835	47.298	60.789	1.00 67.09	С
MOTA	3845	CA	GLY	73	92.443	47.075	61.126	1.00 50.60	C
MOTA	3846	C	ĢLY	73	91.964	45.670	60.808	1.00 56.73	·C
MOTA	3847	0	GLY	73	91.356	45.434	59.760	1.00 64.99	C
ATOM	3848	N	ASN	74	92.246	44.735	61.713	1.00 46.04	C
MOTA	3849	CA	ASN	74	91.828	43.342	61.566	1.00 54.16	C
MOTA	3850	CB	ASN	74	90.316	43.231	61.790	1.00 79.65	С
ATOM	3851	CG	ASN	74	89.953	42.174	62.814	1.00 90.87	C
ATOM	3852	OD1	ASN	74	88.992	42.334	63.574	1.00 90.68	C
ATOM	3853	ND2	ASN	74	90.715	41.086	62.838	1.00 89.35	С
MOTA	3854	C	ASN	74	92.180	42.738	60.215	1.00 54.40	C
MOTA	3855	O 4	ASN	74	93.332	42.413	59.951	1.00 62.07	C
MOTA	3856	\mathbf{N}	GLU	75	91.171	42.577	59.364	1.00 55.88	C
MOTA	3857	CA	GLU	75	91.364	42.010	58.035	1.00 47.09	C
ATOM	3858	CB	GLU	75	90.269	40.988	57.722	1.00 56.56	С
ATOM	3859	CG	GLU	75	88.966	41.211	58.471	1.00 48.68	C
ATOM	3860	CD	GLU	. 75	88.614	40.047	59.379	1.00 58.55	C
MOTA	3861	OE1	GLU	75	88.407	38.928	58.859	1.00 55.16	C
ATOM	3862	OE2	GLU	75	88.547	40.250	60.612	1.00 54.08	C

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MOTA	3863	C	GLU	75	91.323	43.127	57.013	1.00	44.01	C
MOTA	3864	0	GLU	75 [.]	90.606	43.055	56.017	1.00	27.15	C
MOTA	3865	N	SER	76 .	92.107	44.162	57.268	1.00	36.46	, C
ATOM	3866	CA	SER	76	92.143	45.296	56.376	1.00	31.85	C
ATOM	3867	CB	SER	76	90.835	46.072	56.492	1.00	24.92	C
MOTA	3868	OG	SER	76	90.835	46.835	57.681	1.00	16.45	C
ATOM	3869	C	SER	76	93.292	46.208	56.733		32.47	C
ATOM	3870	0	SER	76	93.689	46.294	57.892	1.00	34.00	C
MOTA	3871	N	VAL	77	93.826	46.884	55.723	1.00	38.60	C
MOTA	.3872	CA	VAL	77	94.906	47.848	55.908	1.00	32.38	C
MOTA	3873	CB	VAL '	77	96.272	47.308	55.386		45.71	C
MOTA	3874	CG1	VAL	77 	96.747	48.122	54.190		37.47	C
ATOM	3875	CG2	VAL	77	97.327	47.372	56.484		19.29	C
ATOM	3876	C	VAL	77	94.509	49.083	55.101		33.67	C
MOTA	3877	0	VAL	77	93.934	48.972	54.013		38.06	C
ATOM	3878	N	THR	78	94.811	50.260	55.630		40.03	C
ATOM	3879	CA	THR	78	94.475	51.493	54.929	1.00	38.24	C
ATOM	3880	CB	THR	78	93.548	52.377	55.787	1.00	35.10	C
ATOM	3881	OG1	THR	78	92.594	51.551	56.472		36.53	C
ATOM	3882	CG2	THR	78	92.804	53.363	54.916		36.45	C C
MOTA	3883	C	THR	78 78	95.745	52.269	54.580 55.451	1.00	35.91 31.92	C
MOTA	3884	O	THR	78	96.574	52.540 52.610	53.301		39.13	C
ATOM	3885	N	PHE	79	,95.896 97.059	53.358	52.824		29.89	C
ATOM	3886	CA	PHE	79 70	97.532	52.801	51.487		35.47	C
ATOM	3887	CB	PHE PHE	79 79	97.93 <i>2</i> 97.996	51.380	51.553		41.67	. C
MOTA	3888	CG	PHE	7 <i>9</i> 79	97.174	50.342	51.123		46.33	C
MOTA	3889 3890	CD1 CD2	PHE	7 <i>9</i> 79 .	99.271	51.077	52.019		35.39	C
MOTA MOTA	3891	CE1	PHE	79	97.621	49.026	51.155		34.72	C
ATOM	3892	CE2	PHE	79	99.724	49.765	52.054		17.78	. C
ATOM	3893	CZ	PHE	79	98.895	48.736	51.619		26.82	ď
ATOM	3894	C	PHE	79	96.687	54.816	52.645	1.00	20.01	, C
ATOM	3895	0	PHE	79	95.843	55.143	51.817		39.07	C
ATOM	3896	N	TYR	80	97.328	55.690	53.414		37.92	C
ATOM	3897	CA	TYR	80 '	97.048	57.123	53.361		39.66	C
ATOM	3898	CB	TYR	80	97.043	57.706	54.775	1.00	41.42	С
ATOM	3899	CG	TYR	80	96.541	59.125	54.849	1.00	29.87	C
ATOM	3900	CD1	TYR	80	95.857	59.702	53.782	1.00	31.82	C
ATOM	3901	CE1	TYR	80	95.404	61.008	53.842	1.00	38.26	C
ATOM	3902	CD2	TYR	80	96.756	59.895	55.984	1.00	35.48	C
ATOM	3903	CE2	TYR	80	96.307	61.207	56.060	1.00	38.78	C
MOTA	3904	CZ	TYR	80	95.632	61.758	54.984	1.00	46.52	C
ATOM	3905	ОН	TYR	80	95.195	63.066	55.046	1.00	43.37	C
ATOM	3906	C	TYR	80	98.034	57.901	52.508	1.00	36.43	C.
MOTA	3907	· O	TYR	80	98.960	58.529	53.028	1.00	41.51	C
MOTA	3908	N	LEU	81	97.817	57.873	51.199	1.00	37.66	C
MOTA	3909	CA	LEU	81	98.694	58.576	50.268	1.00	43.35	C
MOTA	3910	CB	LEU	81	98.538	57.997	48.861	1.00	40.97	C
MOTA	3911	CG	LEU	81	98.392	56.485	48.721	1.00	35.20	C
MOTA	3912	CD1	LEU	81	98.068	56.154	47.268	1.00	41.59	C
ATOM	3913	CD2	LEU	81	99.670	55.798	49.141	1.00	34.03	C
ATOM	3914	C	LEU	81	98.457	60.092	50.216	1.00	39.41	C
MOTA	3915	0	LEU	81	97.410	60.552	49.759	1.00	30.90	C

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ATOM	3916	N	GLN	82	99.450	6Ó.853	50.678	1.00 45.56	C
ATOM	3917	CA	GLN	82	99.397	62.315	50.681	1.00 47.39	<u>.</u> C
ATOM	3918	CB	GLN	82	99.884	62.868	52.023	1.00 48.95	C
ATOM	3919	CG	GLN	82	99.479	62.062	53.246	1.00 42.53	C
ATOM	3920	CD	GLN	82	99.397	62.921	54.491	1.00 35.76	C
ATOM	3921	OE1	GLN	82	99.826	62.514	55.575	1.00 35.27	C
MOTA	3922	NE2	GLN	82	98.857	64.127	54.339	1.00 29.92	C.
ATOM	3923	C	GLN	82	100.280	62.884	49.571	1.00 42.88	C
ATOM	3924	0	GLN	82	101.148	62.194	49.035	1.00 41.58	C
ATOM	3925	N	ASN	83	100.060	64.148	49.237	1.00 45.46	C
ATOM	3926	CA	ASN	83	100.843	64.806	48.197	1.00 43.88	C
ATOM	3927	CB	ASN	83	102.229	65.139	48.748	1.00 38.56	C
ATOM	3928	CG	ASN	83	102.170	66.242	49.779	1.00 47.82	C
ATOM	3929	OD1	ASN	83	101.274	67.083	49.735	1.00 46.58	C
ATOM	3930	ND2	ASN	83	103.118	66.249	50.715	1.00 33.98	C
ATOM	3931	С	ASN	83	100.951	63.966	46.933	1.00 37.91	C
ATOM	3932	0	ASN	83	102.045	63.718	46.424	1.00 45.24	C
ATOM	3933	N	LEU	84	99.803	63.535	46.430	1.00 28.03	C
ATOM	3934	CA	LEU	84	99.760	62.723	45.230	1.00 19.39	C
ATOM	3935	CB	LEU	84	98.540	61.802	45.263	1.00 26.73	C
ATOM	3936	CG	LEU	84	98.774	60.341	45.664	1.00 34.93	C
ATOM	3937	CD1	LEU	84	97.483	59.552	45.502	1.00 37.57	C
MOTA	3938	CD2		84	99.877	59.729	44.812	1.00 36.66	С
MOTA	3939	C	LEU	84	99.675	63.650	44.037	1.00 20.07	C
ATOM	3940	0	LEU	84	98.914	64.609	44.049	1.00 31.39	C
ATOM	3941	N	TYR	85	100.460	63.365	43.006	1.00 33.90	C
MOTA	3942	CA	TYR	85	100.464	64.187	41.806	1.00 40.42	C
ATOM	3943	CB	TYR	85	101.840	64.117	41.123	1.00 59.23	. C
ATOM	3944	CG	TYR	85	102.989	64.613	41.980	1.00 61.79	C
ATOM	3945	CD1		85	103.155	65.973	42.242	1.00 63.76	C
ATOM	3946		TYR	85	104.193	66.430°	43.053	1.00 67.56	C
ATOM	3947	CD2		85	103.897	63.717	42.549	1.00 64.22	C
ATOM	3948	CE2	TYR	85	104.938	64.162	43.360	1.00 65.83	C
ATOM	3949	CZ	TYR	85	105.079	65.519	43.610	1.00 70.24	C
ATOM	3950	OH	TYR	85	106.093	65.965	44.428	1.00 73.68	C
ATOM	3951	, C	TYR	85	99.378	63.724	40.841	1.00 33.25	C
ATOM	3952	0	TYR	85	98.880	62.606	40.943	1.00 33.16	C
ATOM	3953	N	VAL	86	99.018	64.598	39.907	1.00 32.80	C
MOTA	3954	CA	VAL	86	97.994	64.297	38.914	1.00 31.92	C
ATOM	3955	CB	VAL	86	97.503	65.600	38.241	1.00 29.33	C
ATOM	3956	CG1	VAL	86	98.476	66.730	38.548	1.00 32.20	C
ATOM	3957	CG2	VAL	86	97.361	65.409	36.743	1.00 34.84	C
MOTA	3958	C	VAL	86	98.504	63.312	37.854	1.00 30.06	C
ATOM	3959	0	VAL	86	97.721	62.621	37.204	1.00 28.12	, C
MOTA	3960	N	ASN	87	99.819	63.246	37.685	1.00 37.39	C
ATOM	3961	CA	ASN	87	100.411	62.330	36.716	1.00 31.78	C
MOTA	3962	CB	ASN	87	101.803	62.811	36.348	1.00 30.37	C
ATOM	3963	CG	ASN	87 .	102.721	62.866	37.542	1.00 15.74	С
ATOM	3964	OD1		87	102.334	62.461	38,631	1.00 26.61	C
ATOM	3965		ASN	87	103.939	63.370	37.350	1.00 44.07	С
ATOM	3966	C	ASN	87	100.504	60.955	37.374	1.00 31.73	C
ATOM	3967	0	ASN	87	100.964	59.981	36.773	1.00 29.36	C
ATOM	3968	N	GLN	88	100.063	60.897	38.627	1.00 33.61	· C
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ATOM	3969	CA	GLN	-88	100.082	59.665	39.402	1.00 24.73	С
ATOM	3970	CB	GLN	88	100.430	59.983	40.871	1.00 26.06	C
MOTA	3971	CG	GLN	. 88	101.721	59.314	41.400	1.00 44.43	· C
ATOM	3972	CD	GLN	88	102.692	60.285	42.081	1.00 36.54	C
ATOM	3973	OE1	GLN	88	102.504	60.675	43.235	1.00 26.99	C
ATOM	3974	NE2	GLN	88	103.743	60.668	41.363	1.00 38.97	С
ATOM	3975	C	GLN	- 88	98.747	58.896	39.322	1.00 26.16	С
ATOM	3976	Ö	GLN	88	98.635	57.805	39.872	1.00 22.71	C
ATOM	3977	N	THR	89	97.735	59.448	38.645	1.00 29.74	C
ATOM	3978	CA	THR	89	96.450	58.742	38.548	1.00 35.51	C
ATOM	3979	CB	THR	89	95.381	59.548	37.786	1.00 23.56	C
MOTA	3980	OG1	THR	89	95.586	59.391	36.381	1.00 37.82	C
ATOM	3981	CG2	THR	89	95.456	61.008	38.140	1.00 8.56	C
MOTA	3982	C	THR	89	96.686	57.434	37.808	1.00 30.57	C
MOTA	3983	0	THR	89	97.222	57.427	36.701	1.00 19.99	С
MOTA	3984	N	ASP	90	96.274	56.326	38.411	1.00 26.02	C
ATOM	3985	CA	ASP	90	96.520	55.032	37.799	1.00 29.88	C
ATOM	3986	CB	ASP	90	98.023	54.758	37.848	1.00 17.27	C
MOTA	3987	CG	ASP	90	98.492	53.857	36.738	1.00 29.31	C
MOTA	3988	OD1	ASP	90	99.661	54.010	36.312	1.00 28.02	C
MOTA	3989	OD2	ASP	90	97.695	53.002	36.299	1.00 35.12	C
MOTA	3990	C	ASP	90	95.774	53.918	38.519	1.00 32.73	C
ATOM	3991	0	ASP	90	94.869	54.181	39.307	1.00 28.33	C
MOTA	3992	N	ILE	91	96.155	52.674	38.234	1.00 33.15	С
MOTA	3993	CA	ILE	91	95.549	51.524	38.891	1.00 29.34	C
ATOM	3994	CB	ILE	91	95.320	50.330	37.960	1.00 19.19	C
MOTA	3995	CG2	ILE	91	93.891	49.803	38.124	1.00 7.46	C
MOTA	3996	CG1	ILE	91	95.613	50.734	36.525	1.00 24.90	C
MOTA	3997	CD1	ILE	91	96.736	49.967	35.904	1.00 37.36	C
MOTA	3998	C	ILE	91	96.539	51.070	39.929	1.00 33.79	, C
MOTA	3999	0	ILE.	91	97.707	50.844	39.615	1.00 35.59	С
MOTA	4000	N	TYR	. 92	96.064	50.948	41.162	1.00 39.40	С
ATOM	4001	CA	TYR	92	96.891	50.521	42.274	1.00 25.36	C
MOTA	4002	CB	TYR	92	96.817	51.555	43.398	1.00 24.66	С
MOTA	4003	CG ·	TYR	92	97.472	52.872	43.039	1.00 27.16	C
ATOM	4004	CD1	TYR	92	98.646	53.282	43.669	1.00 32.14	C
MOTA	4005		TYR	.92	99.265	54.474	43.327	1.00 24.99	C
ATOM	4006	CD2	TYR	92	96.933	53.697	42.051	1.00 24.44	C
MOTA	4007	CE2	TYR	92	97.547	54.896	41.703	1.00 24.44	C
ATOM	4008	CZ	TYR	92	98.712	55.275	42.344	1.00 18.97	C
MOTA	4009	OH	TYR	92	99.332	56.454	42.010	1.00 18.71	C
MOTA	4010	C .	TYR	92	96.381	49.179	42.761	1.00 25.56	C
ATOM	4011	O 	TYR	92	95.173	48.942	42.791	1.00 36.33	C
MOTA	4012	N	PHE	93	97.303	48.298	43.127	1.00 28.40	C
MOTA	4013	CA	PHE	93	96.931	46.984	43.621	1.00 29.94	C
ATOM	4014	CB	PHE	93	97.448	45.893	42.689	1.00 17.97	C
MOTA	4015	CG	PHE	93	97.105	46.113	41.258	1.00 24.43	C
MOTA	4016	CD1	PHE	93	97.978	46.793	40.422	1.00 27.44	C
ATOM	4017	CD2	PHE	93	95.921	45.617	40.733	1.00 30.96	C
MOTA	4018	CE1	PHE	93	97.673	46.973	39.076	1.00 46.97	C
ATOM	4019	CE2	PHE	93	95.610	45.792	39.391	1.00 31.89	C
ATOM	4020	CZ	PHE	93	96.483	46,467	38.562	1.00 33.13	C
ATOM	4021	C	PHE	93	97.470	46.739	45.020	1.00 35.26	C

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ATOM	4022	0	PHE	93	98.635	47.022	45.325	1.00 34.73	C
ATOM	4023	. N ·	CYS	94	96.601	46.209	45.870	1.00 48.06	С
ATOM	4024	CA	CYS	94	96.969	45.907	47.235	1.00 36.83	С
ATOM	4025	С	CYS	94	97.635	44.546	47.284	1.00 31.31	C
ATOM	4026	0	CYS	94	97.397	43.692	46.431	1.00 33.02	C
ATOM	4027	CB	CYS	94	95.738	45.921	48.121	1.00 39.16	C
ATOM	4028	SG	CYS	94	96.102	46.711	49.706	1.00 59.22	. C
ATOM	4029	N	LYS	95	98.475	44.349	48.288	1.00 35.15	C
ATOM	4030	CA	LYS	95	99.194	43.093	48.430	1.00 32.02	C
ATOM	4031	CB	LYS	95	100.593	43.227	47.824	1.00 20.95	C
ATOM	4032	CB	LYS	95	101.265	41.913	47.532	1.00 20.55	C
ATOM	4032	CD	LYS	95	102.720	42.111	47.179	1.00 20.20	C
	4034	CE	LYS	95	103.419	40.772	46.979	1.00 20.20	C
ATOM							46.471		C
ATOM	40,35	NZ	LYS	95 U	104.812	40.931		1.00 47.09	C
ATOM	4'036	C	LYS	95	99.301	42.731	49.896	1.00 29.30	
ATOM	4037	0	LYS	95	99.224	43.602	50.759	1.00 32.79	C
ATOM	4038	N	ILE	96	99.480	41.444	50.172	1.00 24.46	C
ATOM	4039	CA	ILE	96	99.619	40.978	51.542	1.00 19.72	C
ATOM	4040	CB	ILE	96	98.258	40.925	52.251	1.00 14.76	C
ATOM -	4041	CG2	ILE	96	97.299	40.052	51.477	1.00 17.83	C
ATOM	4042	CG1	ILE	96	98.434	40.405	53.673	1.00 17.25	C
MOTA	4043		ILE	96	99.184	41.352	54.570	1.00 5.02	C
MOTA	4044	C ·	ILE	96	100.276	39.599	51.602	1.00 26.57	C
MOTA	4045	0	ILE	96	99.852	38.662	50.916	1.00 34.37	C
MOTA	4046	N	GLU	97	101.321	39.491	52.419	1.00 20.47	С
MOTA	4047	CA	GLU	97	102.052	38.243	52.592	1.00 27.23	С
MOTA	4048	CB	GLU	97	103.367	38.279	51.793	1.00 32.57	C
MOTA	4049	CG	GLU	97	104.186	39.550	51.949	1.00 38.60	С
MOTA	4050	CD	GLU	97	104.535	40.193	50.618	1.00 46.08	C
ATOM	4051	OE1	GLU	. 97	105.239	39.548	49.815	1.00 37.73	C
MOTA	4052	OE2	GLU	97	104.108	41.348	50.379	1.00 54.19	С
MOTA	4053	C	GLU	. 97	102.343	37.951	54.071	1.00 30.22	C
MOTA	4054	O	GLU	97	102.705	38.841	54.844	1.00 27.30	C
MOTA	4055	N	VAL	98	102.158	36.694	54.455	1.00 24.37	C
MOTA	4056	CA	VAL	98	102.395	36.256	55.817	1.00 17.97	C
ATOM	4057	CB	VAL	98	101.361	35.183	56.224	1.00 33.66	G
MOTA	4058	· CG1	VAL	9.8	102.002	34.115	57.113	1.00 46.61	/ C
ATOM	4059	CG2	VAL	98	100.200	35.844	56.931	1.00 31.46	C
ATOM	4060	C	VAL	98	103.787	35.664	55.808	1.00 24.36	C
ATOM	4061	0	VAL	. 98	104.147	34.979	54.858	1.00 17.44	C
MOTA	4062	N	MET	99	104.569	35.936	56.851	1.00 41.56	C
MOTA	4063	CA	MET	· 99	105.932	35.414	56.940	1.00 37.25	C
MOTA	4064	CB	MET	99	106.951	36.540	56.753	1.00 26.44	, C
ATOM	4065	CG	MET	99	106.449	37.906	57.176	1.00 37.71	C
MOTA	4066	SD	MET	99	106.981	39.212	56.039	1.00 49.54	C
MOTA	4067	CE	MET	99	105.587	39.271	54.899	1.00 38.22	C
ATOM	4068	C	MET	99	106.182	34.728	58.273	1.00 37.57	C
ATOM	4069	0	MET	99	107.286	34.241	58.526	1.00 31.40	C
ATOM	4070	N	TYR	100	105.154	34.712	59.119	1.00 45.50	C
ATOM	4071	CA	TYR	100	105.210	34.084	60.439	1.00 45.47	C
MOTA	4072	CB	TYR	100	106.441	34.532	61.218	1.00 49.87	С
MOTA	4073	CG	TYR	100	106.979	33.489	62.176	1.00 54.53	C
ATOM	4074	CD1	TYR	100	107.908	32.545	61.745	1.00 66.10	С
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	ATOM	4075	CE1	TYR	100	* · ·	108.466	31.625	62.622	1.00	67.96	С
	ATOM	4076	CD2	TYR	100		106.611	33.483	63.523 [,]	1.00	50.84	C
	ATOM	4077	CE2	TYR	100		107.166	32.559	64.415	1.00		C
	MOTA	4078	CZ	TYR	100		108.098	31.636	63.951	1.00	57.97	С
	ATOM	4079	ОН	TYR	100		108.687	30.728	64.801	1.00		С
	ATOM	4080	C	TYR	100		103.978	34.429	61.259	1.00		C
	ATOM	4081	·O	TYR	100		103.561	35.587	61.307	1.00	42.87	C
	ATOM	4082	N	PRO	101		103.380	33.422	61.920	1.00		C
	ATOM	4083	CD	PRO	101		102.180	33.528	62.771	1.00	52.41	C
	ATOM	4084	CA	PRO	101		103.902	32.054	61.844	1.00		C
	ATOM	4085	CB	PRO	101		103.126	31.300	62.927	1.00	42.16	C
	ATOM	4086	CG	PRO	101		101.906	32.115	63.189	1.00	38.19	C
	ATOM	4087	C	PRO	101		103.711	31.468	60.441	1.00		C
	MOTA	4088	0	PRO	101		102.901	31.960	59.648	1.00	47.74	Ċ
	ATOM	4089	N	PRO	102		104.455	30.400	60.122	1.00	58.81	C
	ATOM	4090	CD	PRO	102		105.410	29.707	61.000	1.00	43.99	C
	ATOM	4091	CA	PRO	102		104.368	29.758	58.807	1.00	54.29	C
	ATOM	4092	CB	PRO	102		105.585	28.824	58.766	1.00		C
	ATOM	4093	CG	PRO	102 .		106.354	29.090	60.030	1.00	46.28	C
	ATOM	4094	C	PRO	102		103.072	28.997	58.565	1.00		C
	ATOM	4095	0	PRO	102		102.265	28.812	59.475	1.00		, C
	ATOM	4096	N	PRO	103		102.858	28.550	57.321	1.00		C
	ATOM	4097	CD	PRO	103		101.692	27.757	56.901	1.00		C
	ATOM	4098	CA	PRO	103		103.784	28.756	56.209		34.80	C
	ATOM	4099	CB	PRO	103		103.457	27.611	55.247		35.84	C
J	ATOM	4100	CG	PRO	103		102.280	26.863	55.860		31.11	C
	MOTA	4101	C -	PRO	103		103.581	30.127	55.566		39.20	, C
	ATOM	4102	0	PRO	103		102.790	30.939	56.055		35.30	С
	ATOM	4103	N	TYR	104	-	104.311	30.382	54.481		40.51	С
	ATOM	4104	CA	TYR	104		104.199	31.644	53.760	1.00	40.50	C -
	ATOM	4105	CB	TYR	104	F	105.226	31.719	52.630	1.00	34.12	C
	ATOM	4106	CG	TYR	104	,	105.224	33.036	51.888	1.00	35.99	C
	ATOM	4107	CD1	TYR	104		104.659	33.143	50.615	1.00	49.18	C
	ATOM	4108	CE1	TYR	104		104.652	34.363	49.926	1.00		С
	ATOM	4109	CD2	TYR	104		105.784	34.179	52.458	1.00	34.98	C
	ATOM	4110	CE2	TYR	104		105.782	35.403	51.779	1.00	35.62	C
	ATOM	4111	CZ	TYR	104		105.215	35.485	50.518	1.00	39.99	С
	ATOM	4112	OH	TYR	104	•	105.205	36.685	49.853	1.00	32.85	С
	MOTA	4113	C	TYR	104		102.804	31.725	53.168	1.00	44.36	С
	ATOM	4114	0	TYR	104		102.311	30.749	52.603	1.00	46.76	Ċ
	ATOM	4115	N	LEU	105		102.171	32.885	53.304	1.00	47.99	C
	ATOM	4116	CA	LEU	105		100.827	33.096	52.778	1.00	43.06	С
	MOTA	4117	CB	LEU	105		99.859	33.347	53.929	1.00	44.75	C
	MOTA	4118	CG	LEU	105		98.748	32.310	54.097	1.00	55.87	C
	MOTA	4119	CD1	LEU	105		98.181	31.958	52.725	1.00	60.46	С
	ATOM	4120	CD2	LEU	105		99.289	31.062	54.797	1.00	56.52	С
	ATOM	4121	C	LEU	105		100.819	34.283	51.813	1.00	45.31	C
	ATOM	4122	0	LEU	105		101.438	35.308	52.085	1.00	44.10	C
	ATOM	4123	N	ASP	106	ı	100.107	34.144	50.696	1.00	53.21	C
	MOTA	4124	CA	ASP	106		100.046	35.İ99	49.681	1.00	56.65	C
	MOTA	4125	CB	ASP	106		100.961	34.827	48.512	1.00	73.34	С
	MOTA	4126	CG	ASP	106		101.724	36.011	47.979	1.00	81.75	С
	MOTA	4127	OD1	ASP	106		101.437	37.143	48.432	1.00	85.62	C

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ATOM	4128	OD2	ASP	106 ·	102.603	35.802	47.109	1.00 80.61	, C
ATOM	4129	-C	ASP	106	98.639	35.462	49.145	1.00 52.61	C
MOTA	4130	0	ASP	106	97.772	34.592	49.199	1.00 62.59	C
ATOM	4131	N	ASN	107	98.422	36.658	48.609	1.00 42.29	C
ATOM	4132	CA	ASN	107	97.110	37.028	48.072	1.00 50.80	C
MOTA	4133	CB	ASN	107	96.826	38.492	48.359	1.00 42.50	C
ATOM	4134	CG	ASN	107	97 . 855 _,	39.393	47.736	1.00 41.45	C
ATOM	4135	OD1	ASN	107	97.691	39.852	46.607	1.00 44.69	C
MOTA	4136	ND2	ASN	107	98.940	39.637	48.461	1.00 38.52	C
ATOM	4137	C	ASN	107	96.997	36.815	46.564	1.00 55.83	C
MOTA	4138	0	ASN	107	97.990	36.865	45.840	1.00 54.74	C
ATOM	4139	N	GLU	108	95.771	36.601	46.098	1.00 61.82	С
MOTA	4140	CA	GLU	108	95.513	36.393	44.678	1.00 62.32	C
ATOM	4141	CB	GLU	108	94.305	35.474	44.485	1.00 65.84	C
MOTA	4142	CG	GLU	108	93.817	34.809	45.757	1.00 72.69	C
MOTA	4143	CD	GLU	108	92.445	35.295	46.180	1.00 73.87	C
MOTA	4144	OE1	GLU	108	91.534	34.453	46.327	1.00 58.56	C
MOTA	4145	OE2	GLU	108	92.285	36.522	46.366	1.00 79.05	C
MOTA	4146	C	GLU	108	95.244	37.722	43.991	1.00 64.40	C
MOTA	4147	0	GLU	108	94.094	38.171	43.936	1.00 61.70	C
ATOM	4148	N	LYS	109	96.306	38.339	43.467	1.00 64.63	C '
ATOM	4149	CA	LYS	109	96.215	39.629	42.782	1.00 60.84	C
MOTA	4150	CB	LYS	109	,96.054	39.420	41.274	1.00 43.96	C
MOTA	4151	CG	LYS	109	97.094	38.496	40.666	1.00 66.29	C
MOTA	4152	CD	LYS	109	98.399	39.235	40.373	1.00 84.02	C
MOTA	4153	CE	LYS	109	99.309	38.435	39.432	1.00 77.45	. C
ATOM	4154	NZ	LYS	109	100.234	39.299	38.636	1.00 53.39	C
MOTA	4155	C	LYS	109	95.040	40.435	43.331	1.00 59.47	C
MOTA	4156	O ,	LYS	109	94.893	40.571	44.545	1.00 73.09	C
MOTA	4157	N	SER	110	94.201	40.950	42.440	1.00 49.53	C
MOTA	4158	CA	SER	. 110	93.038	41.734	42.841	1.00 50.60	C
MOTA	4159	CB	SER	110	93.404	42.706	43.969	1.00 48.38	C
MOTA	4160	OG	SER	110	93.807	43.962	43.448	1.00 55.94	C
ATOM	4161	C	SER	110	92.455	42.520	41.670	1.00 49.16	C
MOTA	4162	0	SER	110	93.098	42.693	40.634	1.00 36.85	C
ATOM	4163	N	ASN	111	91.228	43.000	41.841	1.00 50.24	
ATOM	4164	CA	ASN	111	90.580	43.770	40.795	1.00 48.26	C '
ATOM	4165	CB	ASN	111	89.073	43.868	41.068	1.00 50.05	C
ATOM	4166	CG	ASN	. 111	88.273	42.770	40.364	1.00 52.55	C
ATOM	4167		ASN	111	87.101	42.539	40.671	1.00 30.90	C
MOTA	4168	ND2	ASN	111	88.912	42.089	39.413		C
MOTA	4169	C	ASN	111 .	91.212	45.162	40.708 39.748	1.00 42.47 1.00 48.01	C
ATOM	4170	O NT	ASN	111	90.982	45.896	41.717	1.00 44.01	C
ATOM	4171	N	GLY	112	92.007 92.682	45.517 46.808	41.729	1.00 44.01	, C
ATOM	4172	CA	GLY	112	91.830	48.015	42.081	1.00 36.58	. C
ATOM	4173	C	GLY	112				1.00 33.31	. C
ATOM	4174	O NT	GLY	112	90.630 92.455	47.892 49.189	42.343 42.094	1.00 33.31	C
ATOM	4175	N	THR	113	92.455	50.416	42.403	.1.00 29.29	C
MOTA	4176	CA	THR	113	91.738	50.416	43.929	1.00 25.84	C
ATOM	4177	CB	THR	113	90.959	51.884	44.186	1.00 23.84	C
ATOM	4178	OG1	THR	113	93.061	50.762	44.514	1.00 15.15	C
ATOM	4179	CG2	THR	113	92.344	51.636	41.722	1.00 33.81	C
MOTA	4180	C	THR	113	<i>74</i> .344	7T.020	#T • 177	4.00 69.94	_

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	MOTA	4181	O'	THR .	113	93.375	52.157	42.133	1.00 21.21	C
	ATOM	4182.	N	ILE	114	91.679	52.074	40.662	1.00 31.79	C
	ATOM	4183	CA	ILE	114	92.093	53.243	39.905	1.00 24.64	C
	ATOM	4184	CB	ILE	114	91.132	53.521	38.721	1.00 29.78	C
	ATOM	4185	CG2	ILE	114	91.159	55.001	38.361	1.00 29.89	C
	ATOM	4186	CG1	ILE	114	91.510	52.661	37.519	1.00 45.18	C
	ATOM	4187	CD1	ILE,	114	91.376	53.376	36.182	1.00 48.49	C
	MOTA	4188	C	ILE	114	92.019	54.450	40.821	1.00 21.71	C
	MOTA	4189	0	ILE	114	91.050	54.632	41.546	1.00 23.04	C
	MOTA	4190	N	ILE	115	93.028	55.296	40.770	1.00 22.63	C
	MOTA	4191	CA	ILE	115	93.003	56.483	41.593	1.00 25.37	C
	MOTA	4192	CB	ILE	115	94.147	56.461	42.585	1.00 19.98	C
	MOTA	4193	CG2	ILE	115	94.249	57.798	43.307	1.00 15.47	. C
	MOTA	4194	CG1	ILE	115	93.925	55.312	43.558	1.00 5.93	. C
	ATOM	4195	CD1	ILE	115	95.089	55.086	44.508	1.00 25.93	C
	ATOM	4196	C	ILE	115	93.104	57.712	40.701	1.00 36.88	C
	MOTA	4197	0	ILE	115	94.147	57.984	40.112	1.00 39.31	C
	ATOM	4198	N	HIS.	116	92.003	58.445	40.604	1.00 36.64	- C
	ATOM	4199	CA	HIS	116	91.951	59.641	39.779	1.00 42.31	C
	MOTA	4200	CB	HIS	116	90.530	59.854	39.250	1.00 55.50	Ç
	ATOM	4201	CG	HIS	116	90.397	61.008	38.303	1.00 53.01	C
	ATOM	4202	CD2	HIS	116	89.311	61.534	37.690	1.00 53.38	C
	ATOM	4203	ND1	HIS	116	,91.473	61.764	37.884	1.00 49.21	C
	ATOM	4204	CE1	HIS	116	91.054	62.700	37.058	1.00 52.55	C
	MOTA	4205	NE2	HIS	116	89.744	62.584	36.920	1.00 46.03	C
	MOTA	4206	C	HIS	116	92.380	60.847	40.592	1.00 38.13	. C
	ATOM	4207	0	HIS	116	91.655	61.278	41.486	1.00 35.69	C
	ATOM	4208	N	VAL	117	93.554	61.387	40.274	1.00 35.30	C
	ATOM	4209	CA	VAL	117	94.078	62.550	40.980	1.00 36.81	C
	MOTA	4210	CB	VAL	117	95.606	62.463	41.146	1.00 24.40	C
	ATOM	4211	CG1	VAL	117	96.075	63.529	42.109	1.00 30.24	C C
	MOTA	4212	CG2	VAL	117	96.004	61.087	41.647	1.00 21.51	C
	ATOM	4213	C	VAL	117	93.747	63.857	40.271	1.00 44.32	C
	ATOM	4214	0	VAL	117	93.901	63.973	39.054	1.00 48.83	C
	ATOM	4215	N	LYS /	118	93.304	64.837	41.055	1.00 61.70	N.*
	ATOM	4216	CA	LYS	118	92.926	66.160	40.555	1.00 65.79 1.00 48.95	. C
	ATOM	4217	CB	LYS	118	94.076	66.809	39.779		
	ATOM	4218	CG	LYS	118	94.137	68.329	39.934	1.00 51.90	, C
	MOTA	4219	CD	LYS	118	93.956	69.065	38.603	1.00 54.76	C
	MOTA	4220	CE	LYS	118	94.163	70.575	38.754	1.00 49.49	C,
•	MOTA	4221	NZ	LYS	118	95.564	71.003	38.435	1.00 45.55 1.00 78.13	C
	ATOM	4222	C	LYS	118	91.693	66.107	39.664		C
7	ATOM	4223	0	LYS	118 .	91.566	67.006	38.807	1.00 88.53 1.00 83.59	C C
	ATOM	4224	OT	LYS	118	90.872	65.178	39.832	T.00 03.33	C
	END						,			

Table 5

DNA sequence of human CD28 cDNA

agactctcag	gccttggcag	gtgcgtcttt	cagttcccct	cacacttcgg	gttcctcggg	60
gaggagggc	tggaacccta	gcccatcgtc	aggacaaaga	tgctcaggct	gctcttggct	120
ctcaacttat	tcccttcaat	tcaagtaaca	ggaaacaaga	ttttggtgaa	gcagtcgccc	180
atgcttgtag	cgtacgacaa	tgcggtcaac	cttagctgca	agtattccta	caatctcttc	240
tcaagggagt	tccgggcatc	ccttcacaaa	ggactggata	gtgctgtgga	agtctgtgtt	300
gtatatggga	attactccca	gcagcttcag	gtttactcaa	aaacggggtt	caactgtgat	360
gggaaattgg	gcaatgaatc	agtgacattc	tacctccaga	atttgtatgt	taaccaaaca	420
gatatttact	tctgcaaaat	tgaagttatg	tatcctcctc	cttacctaga	caatgagaag	480
agcaatggaa	ccattatcca	tgtgaaaggg	aaacaccttt	gtccaagtcc	cctatttccc	540
ggaccttcta	agcccttttg	ggtgctggtg	gtggttggtg	gagtcctggc	ttgctatagc	600
ttgctagtaa	cagtggcctt	tattattttc	tgggtgagga	gtaagaggag	caggctcctg	660
cacagtgact	acatgaacat	gactccccgc	cgccccgggc	ccacccgcaa	gcattaccag	720
ccctatgccc	caccacgcga	cttcgcagcc	tatcgctcct	gacacggacg	cctatccaga	780
agccagccgg	ctggcagccc	ccatctgctc	aatatcactg	ctctggatag	gaaatgaccg	840
ccatctccag	ccggccacct	cagcccctgt	tgggccacca	atgccaattt	ttctcgagtg	900
actagaccaa	atatcaagat	cattttgaga	ctctgaaatg	aagtaaaaga	gatttcctgt	960
gacaggccaa	gtcttacagt	gccatggccc	acattccaac	ttaccatgta	cttagtgact	1020
tgactgagaa	gttagggtag	aaaacaaaaa	gggagtggat	tctgggagcc	tcttcccttt	1080
	tgcacatctc					1140
gaagaaaggc	taggaaatca	ttccttttgg	ttaaatgggt	gtttaatctt	ttggttagtg	1200
ggttaaacgg	ggtaagttag	agtagggga	gggataggaa	gacatattta	aaaaccatta	1260
aaacactgtc	tcccactcat	gaaatgagcc	acgtagttcc	tatttaatgc	tgttttcctt	1320
tagtttagaa	atacatagac	attgtctttt	atgaattctg	atcatattta	gtcattttga	1380
ccaaatgagg	gatttggtca	aatgagggat	tccctcaaag	caatatcagg	taaaccaagt	1440
tgctttcctc	actccctgtc	atgagacttc	agtgttaatg	ttcacaatat	actttcgaaa	1500
gaataaaata	gttc		,	1		1514

Amino acid sequence of human CD28 (SEQ ID NO:1)

MLRLLALNL FPSIQVTGNK ILVKQSPMLV AYDNAVNLSC KYSYNLFSRE FRASLHKGLD SAVEVCVVYG NYSQQLQVYS KTGFNCDGKL GNESVTFYLQ NLYVNQTDIY FCKIEVMYPP PYLDNEKSNG TIIHVKGKHL CPSPLFPGPS KPFWVLVVVG GVLACYSLLV TVAFIIFWVR SKRSRLLHSD YMNMTPRRPG PTRKHYQPYA PPRDFAAYRS

The extracellular domain is shown in bold The stalk region is underlined

Table 6

CD28TFc sequence (SEQ ID NO:2)

(thrombin site separating the two halves of the chimera is shown in bold)

	1		CATC																	:GGCG +	
		GGG	GTAG(GCGA	GTT	'CGT	'CCG	GTG	GTA	CCI	'AAC	CGP	ⁱ CGC	CTI	'GAA	CGA	AAT	AGGF	ACTA	CCGC	
a ·						•			M	D	M	L	R	N	L	L	F	L	M	A	-
	61		GCTC2													GCC				AGCG	
	O L															CGG	•			TCGC	
a		A i	A Q	S	I	N	A	N	K	Ι	L	V	K	Q	s	P	M	L	V	A	-
	101									_						'CTI				GTTC	
	121		CTGT							•						GAA	•			CAAG	
a		Y 1	N C	A	V	N	L	, s	С	K	Y	S	Y	N	L	F	S	R	E	F	_
,	181		GCAT(CCCI	TCA	CAA	AGG	ACT	GGA	TAG	TGC	TGT	GGA	AĞT	'CTG	TGT	'TGI	'ATA'	ATGG	GAAT	240
	1		CGTA	GGA	AGT	'GTT	TCC	TGA	CCI	ATC	ACG	ACA	CCT	'TCA	GAC	ACA	ACA	LATA	ACC	CTTA	
a .′		R I	A S	L	H _.	K	G	L	D	S	A	V	E	V	· C	V	Λ.	Y	G.	N	_
		TAC	rccc	AGCA	GCT	'TCA	GGT	TT	CTC	AAA	AAC	:GGG	GTT	'CAA	CTG	TGA	TGG	GAF	L'L'A	GGGC	, r _
	241		- - :	+- rcgi	CGA	 AGT	+ CCA	 AAT	GAG	TTT	+ TTG'	 JCCC	CAA	-+- GTI.	'GAC	ACT	+	CCTI	TAA	.CCCG	300
a		Y S	5 Q	Q	L	Q	V	Y	S	K	${f T}$	G	F	N ·	С	D	G	K	L	G	-
		AAT	BAAT	CAGT	'GAC	ATT	'CTA	CCI	CCA	GAA	TTT	'GTA	TGT	'TAA	.CCA	AAC	!AGA	· LAT	TTA	CTTC	
	301	TTA	CTTAC	+- 3TCA	CTG	TAA	+ GAT	'GGA	GGT	CTT	++ 'AAA'	.CAI	ACA	-+- TTA	 GGT	TTG	+ TCT	'ATA	LAAT	+ 'GAAG	360
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	261	TG	CAA	'A'Y.T	TGA	AG I	TAI	GLP	TTCC	こましし	TUC	. ≟ ⊥ <i>₽</i> ?	rCCT	AUA.	YCAP.	TTGA	AAD	JAD			TACC	400
	361	AC	GTI	ATT:	-+- ACT	TCA	ATA	CAI	'AGC	 BAGO	AGG	TAA	'GGA	TCI	- + - :GTT	ACI	'CTI	+ 'CTC			+ ATGG	420
a.		C	K	I	E	V	M	Y	P	P	P	Y	L,	Ď	N	E	K	S	N	G	Т	_
	421		TAT	CCA	TGT -+-	'GAA	AGG	GAA	ACF	ACCT	TTC	FTCC	'AAG	TCC	:GCI	LTA:				,	TAAG	480
	124		ATA	.GGT	ACA	CTI	TCC	CTI	TGT	TGGA	LAAC	CAGG	TTC	'AGG	CGA	AAT		•			ATTC	,
a		I	I	H	V	K	G	K	H	L	С	P	S,	P	L	F	P	G	P	S	K	
	481			GGT		CAG	IGGG	TAG	TGG	TAC	;TAA	.+ rGCC	TAG	CAT	'AAG -+-	TAC	'AGT' 	'CCC			ATCA +	540
	~	GG	GGA	.CCA	.TGG	GTC	:CCC	ATC	ACC	CATC	LTA:	'CGG	ATC	GTA	TTC	'ATG	TCA	.GGG	TCT	TCA	TAGT	
a		P	L	V	P	R	G	S	G	S	K	P	S	I	S	T	V	P	E	V	S	***
	541	TC	TGT	CTT	CAT	CTT		+	'AAA		CAA	.GGA	TGT	GCI	'CAÇ	CAT	TAC	TCT	GAC	TCC	TAAG	600
,	2 H T	AG.	ACA	.GAA	GTA	GAA	.GGG	:GGG	TTT	CGG	GTI	ĊCI	'ACA	.CGA	.GTG	GTA	ATG	AGA	.CTG	AGG	ATTC	
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ā.		V	T	C	. V	V	V	D	I	S	K	D	D	P	E	V	Q	·F	S	W	F	•••
	661	GT	AGA	TGA	TGT	GGA	.GGT	'GCA	.CAC	AGC	TCA	GAC	GCA	ACC	CCG	GGA	GGA	GCA	GTT	CAA	CAGC	720
1	OOT	CA'	 TCT	ACT	ACA	CCT	CCA	- .CGT	GTG	 FTCG	AGI	'CTG	CGT	TGG	GGC	CCT	CCT	CGT	CAA	GTT	GTCG	120
a		V	D	D	V	E	V	H	${f T}$	A	Q	T	· Q	P	R	E	E	Q	F	N.	S	·

•	721		TTT	'CC	CTC	'AG'	CAC	TGF	ACT	TCC	CA1	CAI	:GC# 	ACCA	AGGA	ACTG	GCI	'CAA	ATGG	CAA	\GGAG	
	/21		AAA	.GGC	CGAC	FTCF	AGTC	CACI	TGA	AGC	GTA	AGTA	ACGI	.GGT	'CÇI	'GAC	CGA	GTI	ACC	GTI	CCTC	780
a		\mathbf{T}^{*}	F	R	s	V,	S	E	L	P	I	M	H	Q	D	W	L	N	G	K	E	_
	781		CAA	ATG	CAG	GGT	CAA	ACAG	FTGC	'AGC	CTTI	CCC	CTGC	CCC	CAI	'CGA	GAA	AAC	CAT	'CTC	CAAA	
_	701		GTT	'TAC	GTC	CCA	GTT	GTC	ACG	TCG	AAA	\GGG	ACG	:GGG	GTA	GCT	'CTI	TTC	:GTA	GAG	GTTT	840
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CLAIMS

- 1. Method of identifying a modulator of CD28 comprising comparing a structural model of a candidate modulator with a structural model of CD28 to thereby determine whether the modulator will bind to CD28, wherein the structural model is derived from, or comprises, structural coordinates of a crystal of: (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii).
- 2. Method according to claim 1 wherein said comparison comprises fitting (docking) the structural model of the candidate modulator with the structural model of CD28, and optionally determining the binding free energy of binding between the candidate modulator and CD28, wherein a low (more negative) binding free energy indicates that the candidate is likely to bind to CD28.

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- 3. Method according to claim 2 wherein the binding free energy is calculated by
 (i) summing the free energies of interatomic contacts between the structural model of
 the candidate modulator and the structural model of CD28, or
- (ii) determining the free binding energy between the force field of the candidate modulator and the force field of CD28.
- 4. Method according to any one of the preceding claims wherein whether or not the candidate modulator binds to CD28 comprises comparing the fitting of the structural model of the candidate modulator and the structural model of CD28 with the fitting of a structural model of another protein bound to a ligand, to thereby determine whether or not the candidate modulator will bind to CD28.
- 5. Use of the structural coordinates of a crystal of (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii), to identify a modulator of CD28.

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6. Method or use according to any one of the preceding claims wherein the structural coordinates are obtainable by subjecting a crystal of (i) CD28, (ii) a

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fragment of CD28, or (iii) a homologue of (i) or (ii), to X-ray diffraction measurements and deducing the structural coordinates from the diffraction measurements.

- 7. Method or use according to any one of the preceding claims wherein the crystal is of (i), (ii) or (iii) bound to a CD28 specific antibody or a fragment of said antibody.
- 8. Method or use according to any one of the preceding claims wherein the crystal has the structural coordinates shown in Table 4.
 - 9. Method or use according to any one of the preceding claims which further comprises contacting the identified modulator of CD28 with (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of CD28 or the fragment, to determine whether or not the modulator is capable of binding, or modulating the activity of, CD28.
 - 10. A crystal as defined in any one of claims 1, 7 or 8.
- 11. Method of making a crystal as defined in any one of claims 1, 7 or 8

 comprising providing a solution that comprises (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii), and optionally a CD28 specific antibody or fragment of said antibody, and subjecting the solution to conditions that cause the crystal to form.
 - 12. Method according to claim 11 comprising:
 - (a) expressing (i), (ii) or (iii) in the form of a fusion protein with a second protein that is able to form a homodimer, wherein the presence of the second protein in the fusion protein causes (i), (ii) or (iii) to dimerise,
 - (b) cleaving the second protein from the fusion protein,
 - (c) reducing and alkylating one or more of the disulphide bonds present in the stalk-like region of (i), (ii) or (iii), and
 - (d) crystallising (i), (ii) or (iii) bound to a Fab fragment of an antibody.

- 13. Method according to 12 wherein the second protein mentioned in step (b) is an Fc fragment of an antibody.
- 14. Method according to any one of claims 11 to 13 wherein prior to crystallisation (i), (ii) or (iii) is expressed in the form of a fusion protein with an Fc fragment of an antibody, and optionally (i), (ii) or (iii) is cleaved from the fusion protein by thrombin.
- 15. Method according to any one of claims 11 to 14 wherein the (i), (ii) or (iii) is present in monomeric form in the crystal and/or one or more cysteine residues in the stalk-like region of (i), (ii) or (iii) are ethylated in the crystal.
- 16. A machine-readable data storage medium comprising a data storage material encoded with a machine readable data which when read by an appropriate machine is capable of displaying a representation of a crystal as defined in claim 1, 7 or 8.
 - 17. A computer program comprising program code means for performing the method or use of any one of claims 1 to 9 when said program is run on a computer.

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- 18. A computer program product comprising program code means stored on a computer readable storage medium for performing the method or use of any one of claims 1 to 9 when the said program product is run on a computer.
- 19. An antibody that induces superagonistic signalling by a cell surface receptor, wherein said antibody binds to the extracellular portion of the receptor at a membrane proximal region and said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, wherein said antibody does not bind only the C'-D loop of human CD28.
 - 20. A chimeric protein that induces superagonistic signalling by a cell surface receptor, which chimeric protein comprises

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- (i) sequence representing a fragment of a ligand of the receptor, or a homologue of such a fragment, wherein the fragment or homologue is capable of binding to the extracellular portion of the receptor at a membrane proximal region, and (ii) an Fc region of an antibody,
- wherein said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.
 - 21. A chimeric protein that induces superagonistic signalling by one or two types of cell surface receptor, which chimeric protein comprises two Fv regions of an antibody that may be the same or different, wherein at least one of the Fv regions is capable of binding to a first receptor, and the other Fv region either binds to (i) said first receptor, or (ii) a second type of cell surface receptor which is found on a cell that contacts a cell which expresses (i), wherein said first receptor, and optionally also said second receptor, comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.
 - 22. An antibody or chimeric protein according to any one of claims 19 to 21 which
 - (i) binds orthogonally to the main axis of the domain of the receptor which it is binding, and/or
 - (ii) which lies parallel to the cell surface when bound to the receptor, and/or
 - (iii) which binds to a β-strand polypeptide chain of the receptor, and/or
 - (iv) which binds within 75Å of the cell surface.
 - 23. An antibody or chimeric protein according to any one of claims 19 to 22 which binds to a sequence as shown in Table 1 or an equivalent homologous sequence in the proximal membrane region of a receptor which is capable of being induced to signal by the antibody or chimeric protein.
 - 24. An antibody or chimeric protein according to any one of claims 19 to 23 wherein said receptor
 - (i) comprises an ITAM motif, ITIM motif or "switch" signalling motif, and/or

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- (ii) is a member of the CD28 family of proteins, and/or
- (iii) is expressed on the surface of a cell of the immune system, and/or
- (iv) comprises a cytoplasmic domain capable of being phosphorylated by a Src kinase, and/or
- 5 (v) comprises a cytoplasmic domain capable of being dephosphorylated by CD45, and/or
 - (vi) is one of the receptors listed in Table 2, or is a homologue thereof.
- 25. Method of obtaining an agent capable of inducing superagonistic signalling
 by a receptor as defined in claim 20 or 24, comprising determining whether a
 candidate agent binds to a membrane proximal extracellular region of the receptor, to
 thereby determine whether the candidate agent is capable of superagonising the
 receptor.
 - 26. Method according to claim 25 comprising determining whether a candidate agent which binds to the receptor, fails to bind to a mutated version of the receptor wherein one or more amino acids in a membrane proximal extracellular region of the receptor have been mutated, failure to bind to the mutant receptor indicating that the agent is capable of inducing superagonistic signalling by the receptor.
 - 27. Method according to claim 25 or 26 wherein the method is performed by contacting the candidate agent with (i) a full length receptor with said mutations, or (ii) a homologue of (i) with said mutations, or (iii) a fragment of (i) or (ii) comprising said mutations.
 - 28. Method according to claim 25 wherein the location of the binding of the candidate agent is determined by contacting the candidate agent with a peptide which comprises sequence from a membrane proximal extracellular region of the receptor and determining whether the candidate agent binds to the peptide, the binding of the candidate agent to a peptide indicating that the agent is capable of inducing superagonistic signalling by the receptor, wherein said sequence is at least 5 amino acids in length.

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- 29. Method according to claim 28 comprising contacting the candidate agent with an array of overlapping peptides, which peptides represent fragments of the receptor and are 5 to 20 amino acids in length, the binding of the candidate agent to a peptide which represents a membrane proximal extracellular region of the receptor indicating that the agent is capable of inducing superagonistic signalling by the receptor.
- 30. Method of obtaining a superagonistic antibody as defined in any one of claims 19 or 22 to 24 comprising
- (i) screening antibodies for the ability to induce superagonistic signalling by a receptor according to claim 20 or 24, wherein said antibodies have been obtained by immunizing an animal with (a) said receptor, (b) a homologue of said receptor, or (c) a fragment of (a) or (b), or
 - (ii) screening antibodies for the ability to induce superagonistic signalling by a receptor according to claim 20 or 24, wherein said antibodies have been generated in a combinatorial antibody library.
 - 31. Method of obtaining a superagonistic antibody as defined in any one of claims 19 or 22 to 24 comprising
- 20 (i) immunising an animal with a peptide comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor and obtaining the antibody produced by the animal against said sequence, or (ii) selecting an antibody from a combinatorial antibody library based on its ability to bind a peptide as defined in (i), and optionally
 - (iii) recombinantly expressing the antibody obtained in (i) or (ii).
 - 32. Method according to any one of claims 1 to 9 or 25 to 31 further comprising formulating the identified modulator, obtained antibody or obtained agent into a pharmaceutical composition.
 - 33. A peptide of length 5 to 20 amino acids comprising a sequence that binds to an antibody according to any one of claims 19 or 22 to 24.

- 34. Method of inducing superagonistic signalling by a receptor according to claim 20 or 24 on a cell surface comprising sterically inhibiting contact between a phosphatase of the cell and the receptor, excluding a method in which an antibody that binds only the C'-D loop of CD28 is used to sterically inhibit contact between CD28 and the phosphatase CD45.
 - 35. Method of modulating the immune response of a patient comprising administering to the patient:
- (i) a modulator identified by the method of any one of claims 1 to 9, or
 - (ii) an antibody or chimeric protein according to any one of claims 19 to 24 or which is obtained by the method of claim 30 or 31; or
 - (iii) an agent obtained by the method of any one of claims 25 to 29, or
 - (iv) a peptide that stimulates an antibody response in the patient, wherein the
- antibody response comprises an antibody according to any one of claims 19 or 22 to 24, or
 - (vii) a nucleic acid capable of expressing (i), (ii), (iii) or (iv).

Figure 1

A. Superagonistic antibody signalling in vitro

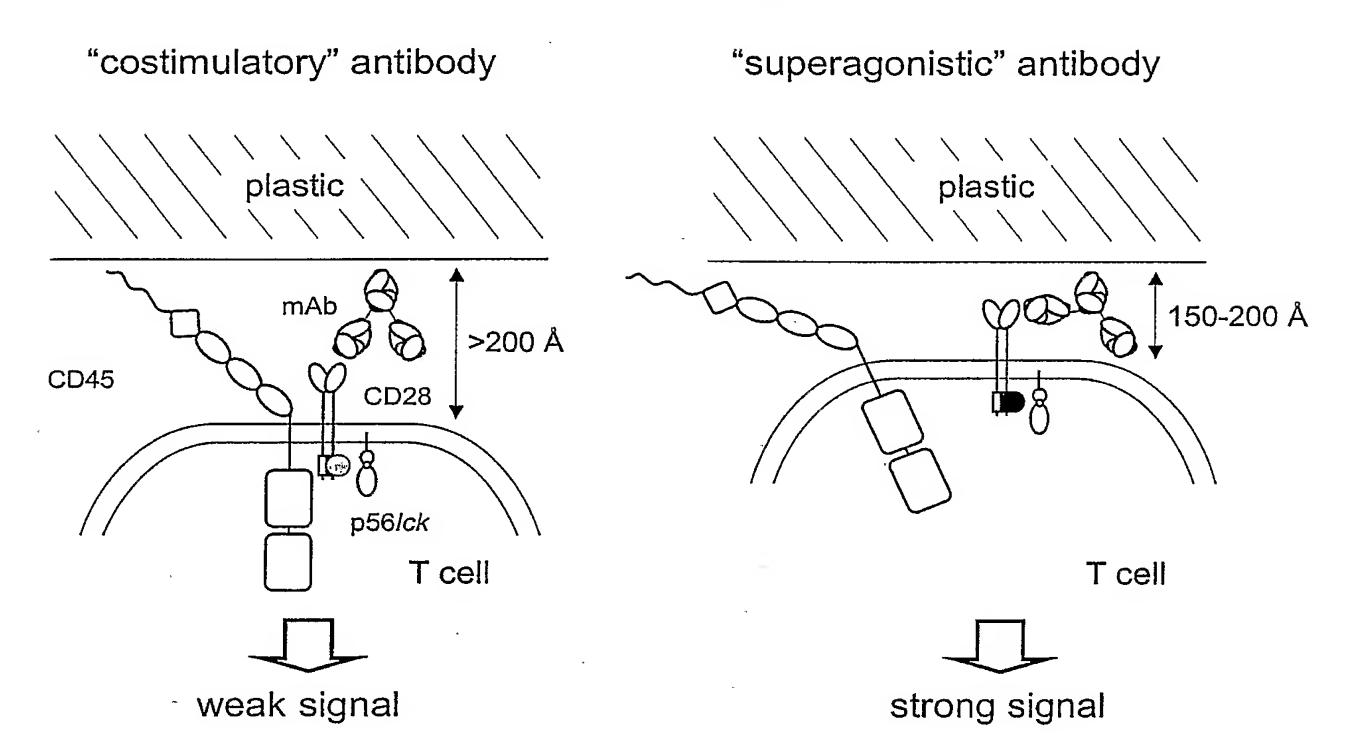


Figure 1

B. Superagonistic antibody signalling in vivo

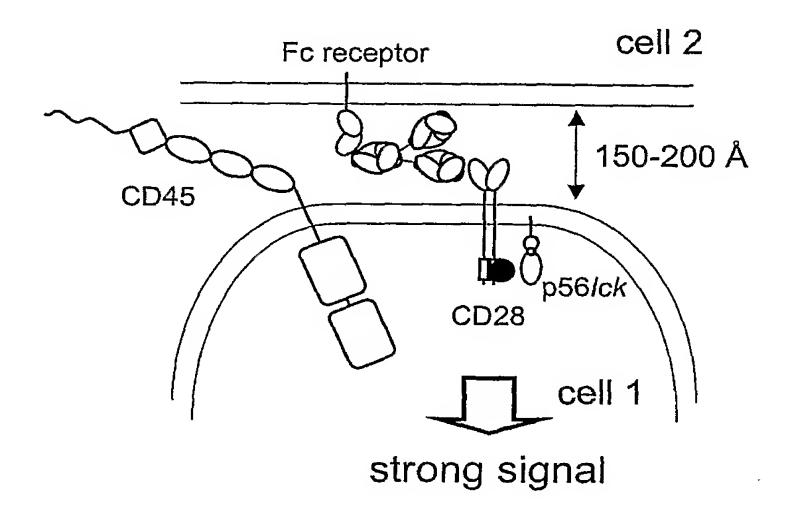
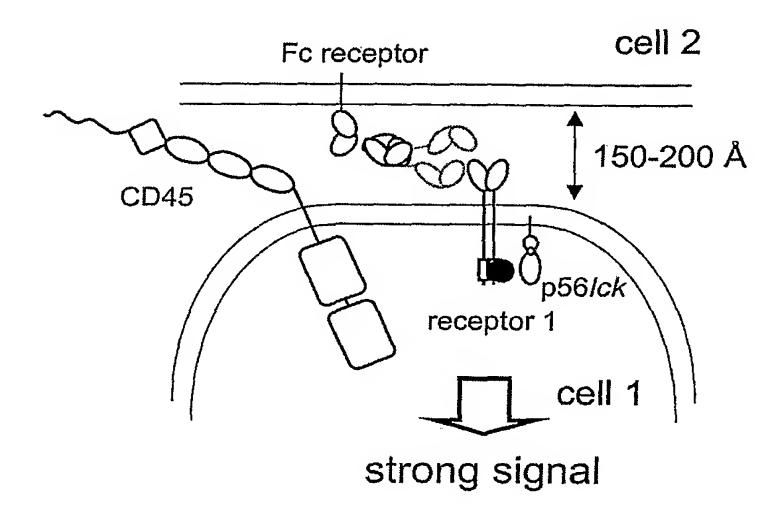


Figure 1

C. Chimeric protein 1 (ligand-based)



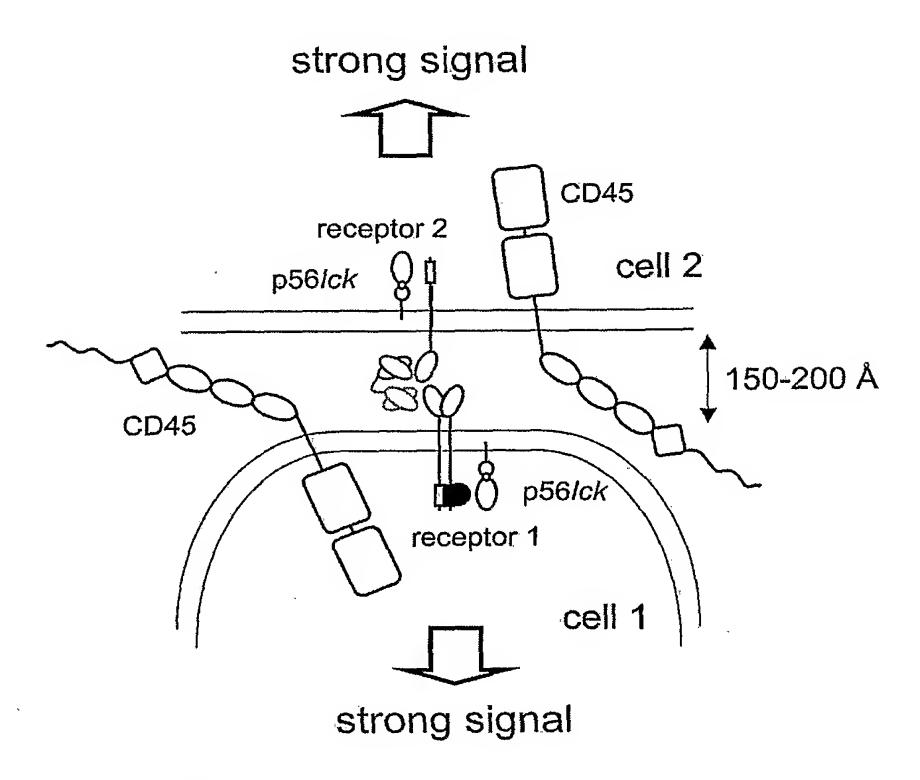


chimeric ligand/Fc superagonist:

 binds Fc receptor on cell 1 and receptor 2 on cell 2

Figure 1

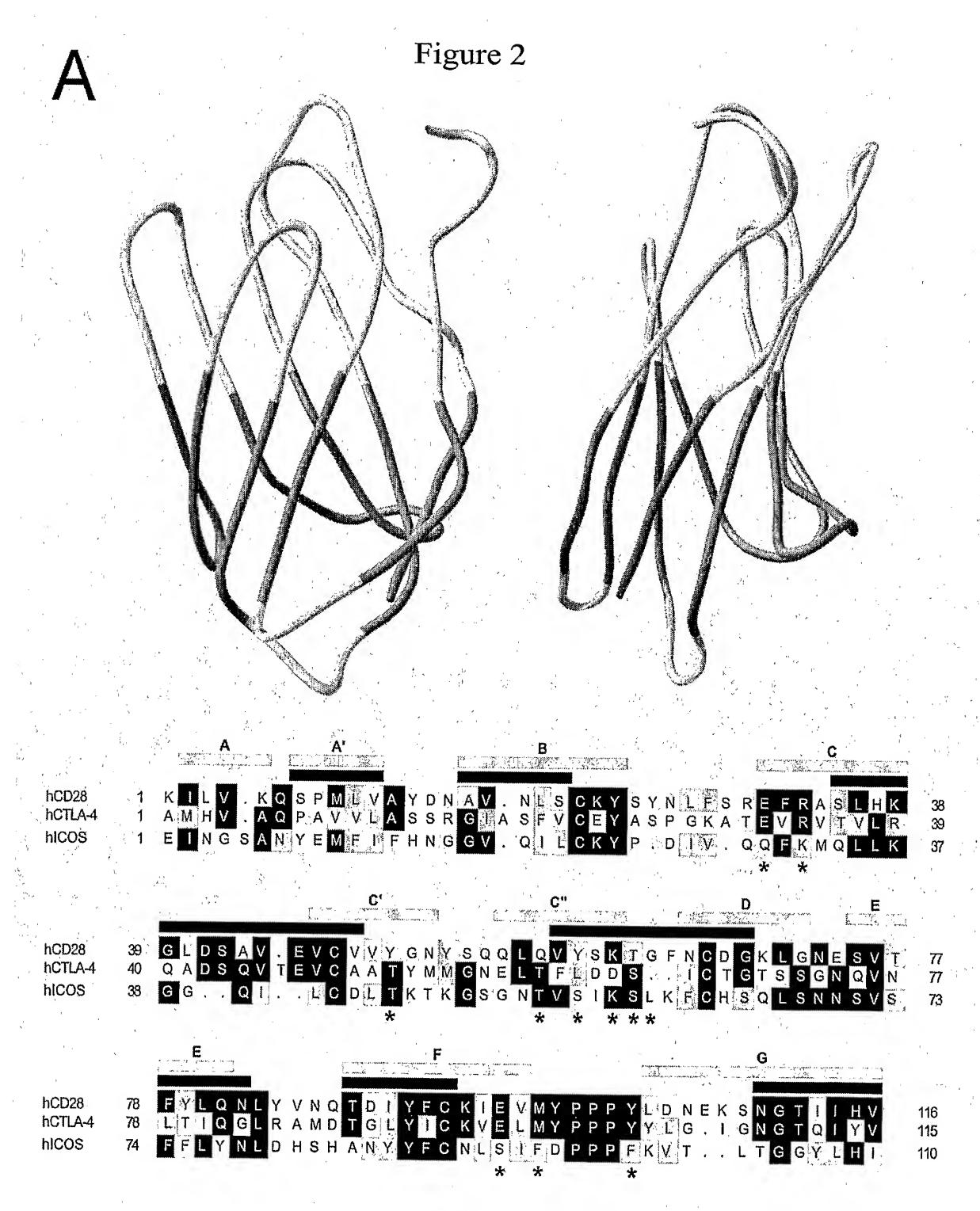
D. Chimeric protein 2 (Fv-based)



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chimeric Fv superagonist:

 binds receptor 1 on cell 1 and receptor 2 on cell 2



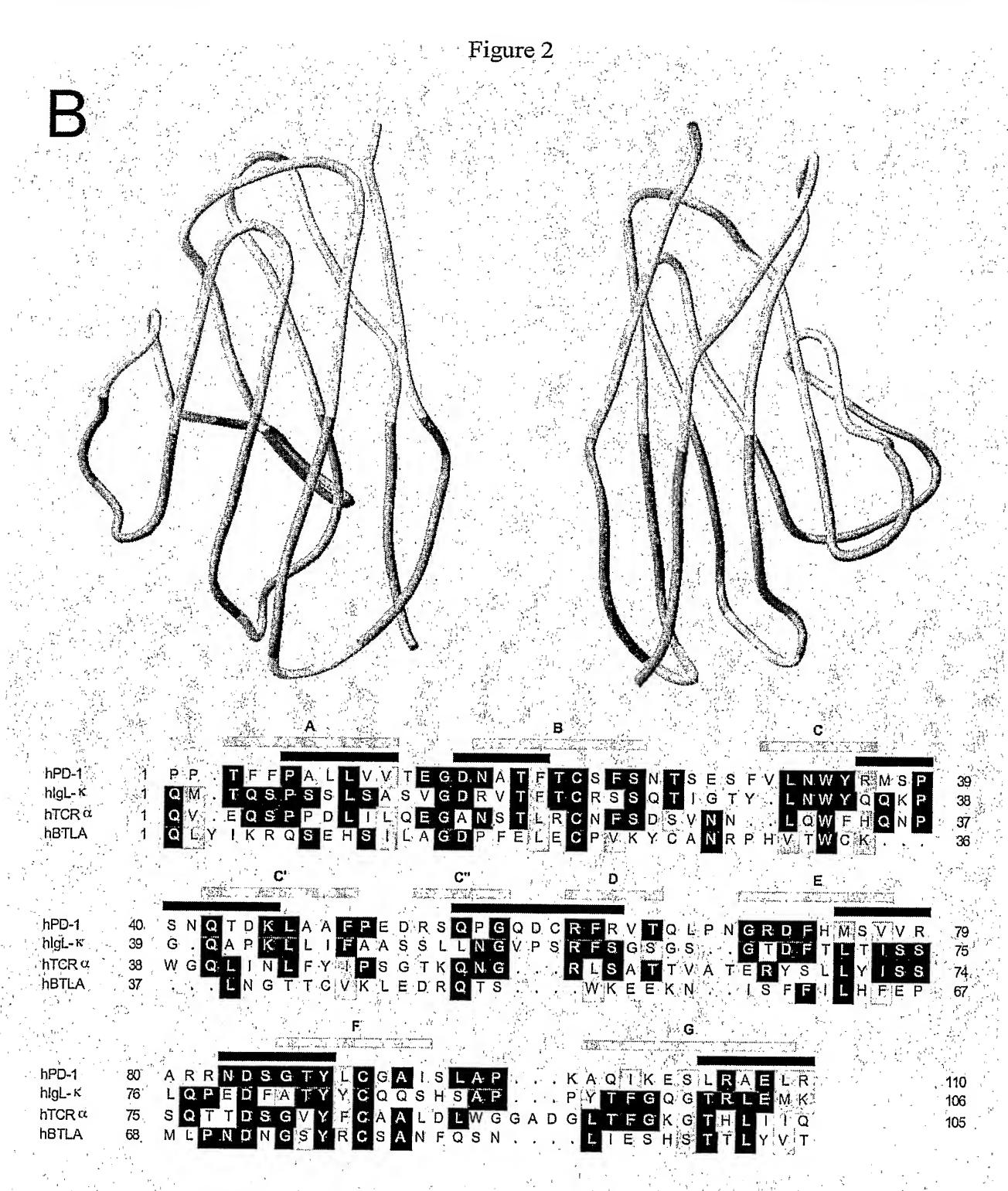


Figure 2

